



Full wwPDB EM Validation Report ⓘ

May 2, 2026 – 01:17 PM EDT

PDB ID : 9P3Y / pdb_00009p3y
EMDB ID : EMD-71259
Title : Andes virus glycoprotein tetramer in complex with ADI-65534 Fab
Authors : McFadden, E.; Guo, L.; McLellan, J.S.
Deposited on : 2025-06-14
Resolution : 3.30 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

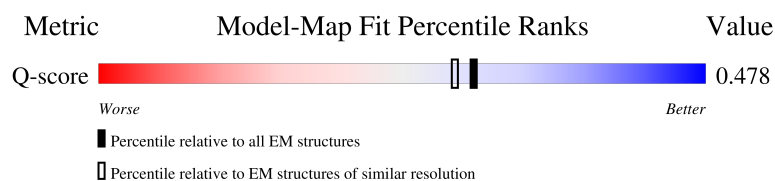
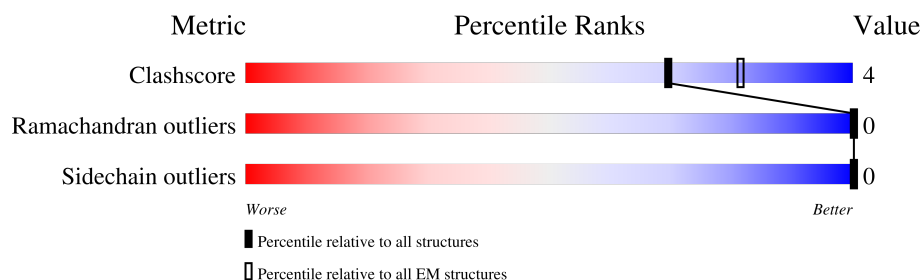
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



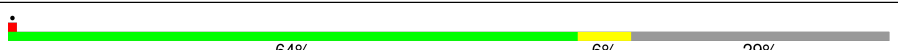
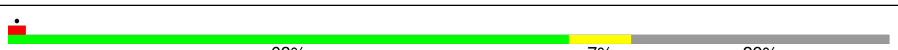
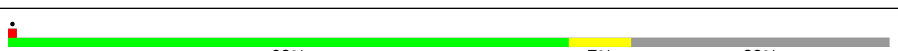
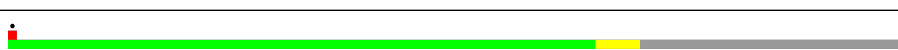
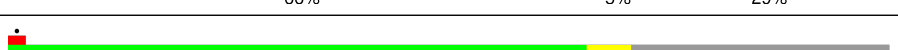
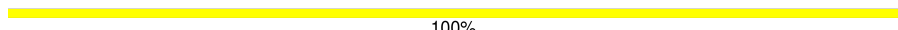
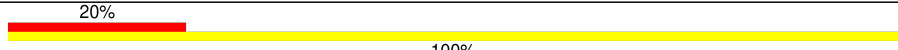
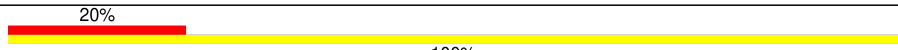
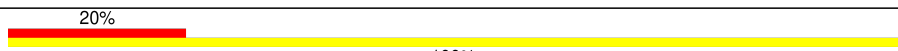
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	I	126	
1	K	126	
1	M	126	
1	O	126	

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Mol	Chain	Length	Quality of chain
2	J	111	
2	L	111	
2	N	111	
2	P	111	
3	A	651	
3	C	651	
3	E	651	
3	G	651	
4	B	609	
4	D	609	
4	F	609	
4	H	609	
5	Q	5	
5	S	5	
5	U	5	
5	W	5	
6	R	2	
6	T	2	
6	V	2	
6	X	2	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 34636 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ADI-65534 variable heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	117	Total	C	N	O	S	0	0
			917	587	157	168	5		
1	K	117	Total	C	N	O	S	0	0
			917	587	157	168	5		
1	M	117	Total	C	N	O	S	0	0
			917	587	157	168	5		
1	O	117	Total	C	N	O	S	0	0
			917	587	157	168	5		

- Molecule 2 is a protein called ADI-65534 variable light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	108	Total	C	N	O	S	0	0
			820	520	137	159	4		
2	L	108	Total	C	N	O	S	0	0
			820	520	137	159	4		
2	N	108	Total	C	N	O	S	0	0
			820	520	137	159	4		
2	P	108	Total	C	N	O	S	0	0
			820	520	137	159	4		

- Molecule 3 is a protein called Glycoprotein N.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	460	Total	C	N	O	S	0	0
			3523	2227	583	683	30		
3	C	460	Total	C	N	O	S	0	0
			3523	2227	583	683	30		
3	E	460	Total	C	N	O	S	0	0
			3523	2227	583	683	30		
3	G	460	Total	C	N	O	S	0	0
			3523	2227	583	683	30		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	535	LYS	VAL	engineered mutation	UNP Q9E006
C	535	LYS	VAL	engineered mutation	UNP Q9E006
E	535	LYS	VAL	engineered mutation	UNP Q9E006
G	535	LYS	VAL	engineered mutation	UNP Q9E006

- Molecule 4 is a protein called Glycoprotein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	431	Total	C	N	O	S	0	0
			3296	2065	553	644	34		
4	D	431	Total	C	N	O	S	0	0
			3296	2065	553	644	34		
4	F	431	Total	C	N	O	S	0	0
			3296	2065	553	644	34		
4	H	431	Total	C	N	O	S	0	0
			3296	2065	553	644	34		

There are 492 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1096	LEU	SER	engineered mutation	UNP Q9E006
B	1139	GLY	-	expression tag	UNP Q9E006
B	1140	SER	-	expression tag	UNP Q9E006
B	1141	GLY	-	expression tag	UNP Q9E006
B	1142	SER	-	expression tag	UNP Q9E006
B	1143	ALA	-	expression tag	UNP Q9E006
B	1144	LEU	-	expression tag	UNP Q9E006
B	1145	PRO	-	expression tag	UNP Q9E006
B	1146	GLY	-	expression tag	UNP Q9E006
B	1147	ASN	-	expression tag	UNP Q9E006
B	1148	PRO	-	expression tag	UNP Q9E006
B	1149	ASP	-	expression tag	UNP Q9E006
B	1150	HIS	-	expression tag	UNP Q9E006
B	1151	ARG	-	expression tag	UNP Q9E006
B	1152	GLU	-	expression tag	UNP Q9E006
B	1153	MET	-	expression tag	UNP Q9E006
B	1154	GLY	-	expression tag	UNP Q9E006
B	1155	GLU	-	expression tag	UNP Q9E006
B	1156	THR	-	expression tag	UNP Q9E006
B	1157	LEU	-	expression tag	UNP Q9E006
B	1158	PRO	-	expression tag	UNP Q9E006
B	1159	GLU	-	expression tag	UNP Q9E006
B	1160	GLU	-	expression tag	UNP Q9E006

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1161	VAL	-	expression tag	UNP Q9E006
B	1162	GLY	-	expression tag	UNP Q9E006
B	1163	GLU	-	expression tag	UNP Q9E006
B	1164	TYR	-	expression tag	UNP Q9E006
B	1165	ARG	-	expression tag	UNP Q9E006
B	1166	GLN	-	expression tag	UNP Q9E006
B	1167	PRO	-	expression tag	UNP Q9E006
B	1168	SER	-	expression tag	UNP Q9E006
B	1169	GLY	-	expression tag	UNP Q9E006
B	1170	GLY	-	expression tag	UNP Q9E006
B	1171	SER	-	expression tag	UNP Q9E006
B	1172	VAL	-	expression tag	UNP Q9E006
B	1173	PRO	-	expression tag	UNP Q9E006
B	1174	VAL	-	expression tag	UNP Q9E006
B	1175	SER	-	expression tag	UNP Q9E006
B	1176	PRO	-	expression tag	UNP Q9E006
B	1177	GLY	-	expression tag	UNP Q9E006
B	1178	PRO	-	expression tag	UNP Q9E006
B	1179	PRO	-	expression tag	UNP Q9E006
B	1180	SER	-	expression tag	UNP Q9E006
B	1181	GLY	-	expression tag	UNP Q9E006
B	1182	LEU	-	expression tag	UNP Q9E006
B	1183	GLU	-	expression tag	UNP Q9E006
B	1184	PRO	-	expression tag	UNP Q9E006
B	1185	THR	-	expression tag	UNP Q9E006
B	1186	SER	-	expression tag	UNP Q9E006
B	1187	SER	-	expression tag	UNP Q9E006
B	1188	SER	-	expression tag	UNP Q9E006
B	1189	PRO	-	expression tag	UNP Q9E006
B	1190	TYR	-	expression tag	UNP Q9E006
B	1191	GLY	-	expression tag	UNP Q9E006
B	1192	GLY	-	expression tag	UNP Q9E006
B	1193	GLY	-	expression tag	UNP Q9E006
B	1194	SER	-	expression tag	UNP Q9E006
B	1195	PHE	-	expression tag	UNP Q9E006
B	1196	ASN	-	expression tag	UNP Q9E006
B	1197	SER	-	expression tag	UNP Q9E006
B	1198	SER	-	expression tag	UNP Q9E006
B	1199	ILE	-	expression tag	UNP Q9E006
B	1200	ASN	-	expression tag	UNP Q9E006
B	1201	ASN	-	expression tag	UNP Q9E006
B	1202	ILE	-	expression tag	UNP Q9E006

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1203	HIS	-	expression tag	UNP Q9E006
B	1204	GLU	-	expression tag	UNP Q9E006
B	1205	MET	-	expression tag	UNP Q9E006
B	1206	GLU	-	expression tag	UNP Q9E006
B	1207	ILE	-	expression tag	UNP Q9E006
B	1208	GLN	-	expression tag	UNP Q9E006
B	1209	LEU	-	expression tag	UNP Q9E006
B	1210	LYS	-	expression tag	UNP Q9E006
B	1211	ASP	-	expression tag	UNP Q9E006
B	1212	ALA	-	expression tag	UNP Q9E006
B	1213	LEU	-	expression tag	UNP Q9E006
B	1214	GLU	-	expression tag	UNP Q9E006
B	1215	LYS	-	expression tag	UNP Q9E006
B	1216	ASN	-	expression tag	UNP Q9E006
B	1217	GLN	-	expression tag	UNP Q9E006
B	1218	GLN	-	expression tag	UNP Q9E006
B	1219	TRP	-	expression tag	UNP Q9E006
B	1220	LEU	-	expression tag	UNP Q9E006
B	1221	VAL	-	expression tag	UNP Q9E006
B	1222	TYR	-	expression tag	UNP Q9E006
B	1223	ASP	-	expression tag	UNP Q9E006
B	1224	GLN	-	expression tag	UNP Q9E006
B	1225	GLN	-	expression tag	UNP Q9E006
B	1226	ARG	-	expression tag	UNP Q9E006
B	1227	GLU	-	expression tag	UNP Q9E006
B	1228	VAL	-	expression tag	UNP Q9E006
B	1229	TYR	-	expression tag	UNP Q9E006
B	1230	VAL	-	expression tag	UNP Q9E006
B	1231	LYS	-	expression tag	UNP Q9E006
B	1232	GLY	-	expression tag	UNP Q9E006
B	1233	LEU	-	expression tag	UNP Q9E006
B	1234	LEU	-	expression tag	UNP Q9E006
B	1235	ALA	-	expression tag	UNP Q9E006
B	1236	LYS	-	expression tag	UNP Q9E006
B	1237	ILE	-	expression tag	UNP Q9E006
B	1238	PHE	-	expression tag	UNP Q9E006
B	1239	GLU	-	expression tag	UNP Q9E006
B	1240	LEU	-	expression tag	UNP Q9E006
B	1241	GLU	-	expression tag	UNP Q9E006
B	1242	LYS	-	expression tag	UNP Q9E006
B	1243	LYS	-	expression tag	UNP Q9E006
B	1244	THR	-	expression tag	UNP Q9E006

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1245	GLU	-	expression tag	UNP Q9E006
B	1246	THR	-	expression tag	UNP Q9E006
B	1247	ALA	-	expression tag	UNP Q9E006
B	1248	ALA	-	expression tag	UNP Q9E006
B	1249	GLY	-	expression tag	UNP Q9E006
B	1250	GLY	-	expression tag	UNP Q9E006
B	1251	GLY	-	expression tag	UNP Q9E006
B	1252	SER	-	expression tag	UNP Q9E006
B	1253	HIS	-	expression tag	UNP Q9E006
B	1254	HIS	-	expression tag	UNP Q9E006
B	1255	HIS	-	expression tag	UNP Q9E006
B	1256	HIS	-	expression tag	UNP Q9E006
B	1257	HIS	-	expression tag	UNP Q9E006
B	1258	HIS	-	expression tag	UNP Q9E006
B	1259	HIS	-	expression tag	UNP Q9E006
B	1260	HIS	-	expression tag	UNP Q9E006
D	1096	LEU	SER	engineered mutation	UNP Q9E006
D	1139	GLY	-	expression tag	UNP Q9E006
D	1140	SER	-	expression tag	UNP Q9E006
D	1141	GLY	-	expression tag	UNP Q9E006
D	1142	SER	-	expression tag	UNP Q9E006
D	1143	ALA	-	expression tag	UNP Q9E006
D	1144	LEU	-	expression tag	UNP Q9E006
D	1145	PRO	-	expression tag	UNP Q9E006
D	1146	GLY	-	expression tag	UNP Q9E006
D	1147	ASN	-	expression tag	UNP Q9E006
D	1148	PRO	-	expression tag	UNP Q9E006
D	1149	ASP	-	expression tag	UNP Q9E006
D	1150	HIS	-	expression tag	UNP Q9E006
D	1151	ARG	-	expression tag	UNP Q9E006
D	1152	GLU	-	expression tag	UNP Q9E006
D	1153	MET	-	expression tag	UNP Q9E006
D	1154	GLY	-	expression tag	UNP Q9E006
D	1155	GLU	-	expression tag	UNP Q9E006
D	1156	THR	-	expression tag	UNP Q9E006
D	1157	LEU	-	expression tag	UNP Q9E006
D	1158	PRO	-	expression tag	UNP Q9E006
D	1159	GLU	-	expression tag	UNP Q9E006
D	1160	GLU	-	expression tag	UNP Q9E006
D	1161	VAL	-	expression tag	UNP Q9E006
D	1162	GLY	-	expression tag	UNP Q9E006
D	1163	GLU	-	expression tag	UNP Q9E006

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1164	TYR	-	expression tag	UNP Q9E006
D	1165	ARG	-	expression tag	UNP Q9E006
D	1166	GLN	-	expression tag	UNP Q9E006
D	1167	PRO	-	expression tag	UNP Q9E006
D	1168	SER	-	expression tag	UNP Q9E006
D	1169	GLY	-	expression tag	UNP Q9E006
D	1170	GLY	-	expression tag	UNP Q9E006
D	1171	SER	-	expression tag	UNP Q9E006
D	1172	VAL	-	expression tag	UNP Q9E006
D	1173	PRO	-	expression tag	UNP Q9E006
D	1174	VAL	-	expression tag	UNP Q9E006
D	1175	SER	-	expression tag	UNP Q9E006
D	1176	PRO	-	expression tag	UNP Q9E006
D	1177	GLY	-	expression tag	UNP Q9E006
D	1178	PRO	-	expression tag	UNP Q9E006
D	1179	PRO	-	expression tag	UNP Q9E006
D	1180	SER	-	expression tag	UNP Q9E006
D	1181	GLY	-	expression tag	UNP Q9E006
D	1182	LEU	-	expression tag	UNP Q9E006
D	1183	GLU	-	expression tag	UNP Q9E006
D	1184	PRO	-	expression tag	UNP Q9E006
D	1185	THR	-	expression tag	UNP Q9E006
D	1186	SER	-	expression tag	UNP Q9E006
D	1187	SER	-	expression tag	UNP Q9E006
D	1188	SER	-	expression tag	UNP Q9E006
D	1189	PRO	-	expression tag	UNP Q9E006
D	1190	TYR	-	expression tag	UNP Q9E006
D	1191	GLY	-	expression tag	UNP Q9E006
D	1192	GLY	-	expression tag	UNP Q9E006
D	1193	GLY	-	expression tag	UNP Q9E006
D	1194	SER	-	expression tag	UNP Q9E006
D	1195	PHE	-	expression tag	UNP Q9E006
D	1196	ASN	-	expression tag	UNP Q9E006
D	1197	SER	-	expression tag	UNP Q9E006
D	1198	SER	-	expression tag	UNP Q9E006
D	1199	ILE	-	expression tag	UNP Q9E006
D	1200	ASN	-	expression tag	UNP Q9E006
D	1201	ASN	-	expression tag	UNP Q9E006
D	1202	ILE	-	expression tag	UNP Q9E006
D	1203	HIS	-	expression tag	UNP Q9E006
D	1204	GLU	-	expression tag	UNP Q9E006
D	1205	MET	-	expression tag	UNP Q9E006

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1206	GLU	-	expression tag	UNP Q9E006
D	1207	ILE	-	expression tag	UNP Q9E006
D	1208	GLN	-	expression tag	UNP Q9E006
D	1209	LEU	-	expression tag	UNP Q9E006
D	1210	LYS	-	expression tag	UNP Q9E006
D	1211	ASP	-	expression tag	UNP Q9E006
D	1212	ALA	-	expression tag	UNP Q9E006
D	1213	LEU	-	expression tag	UNP Q9E006
D	1214	GLU	-	expression tag	UNP Q9E006
D	1215	LYS	-	expression tag	UNP Q9E006
D	1216	ASN	-	expression tag	UNP Q9E006
D	1217	GLN	-	expression tag	UNP Q9E006
D	1218	GLN	-	expression tag	UNP Q9E006
D	1219	TRP	-	expression tag	UNP Q9E006
D	1220	LEU	-	expression tag	UNP Q9E006
D	1221	VAL	-	expression tag	UNP Q9E006
D	1222	TYR	-	expression tag	UNP Q9E006
D	1223	ASP	-	expression tag	UNP Q9E006
D	1224	GLN	-	expression tag	UNP Q9E006
D	1225	GLN	-	expression tag	UNP Q9E006
D	1226	ARG	-	expression tag	UNP Q9E006
D	1227	GLU	-	expression tag	UNP Q9E006
D	1228	VAL	-	expression tag	UNP Q9E006
D	1229	TYR	-	expression tag	UNP Q9E006
D	1230	VAL	-	expression tag	UNP Q9E006
D	1231	LYS	-	expression tag	UNP Q9E006
D	1232	GLY	-	expression tag	UNP Q9E006
D	1233	LEU	-	expression tag	UNP Q9E006
D	1234	LEU	-	expression tag	UNP Q9E006
D	1235	ALA	-	expression tag	UNP Q9E006
D	1236	LYS	-	expression tag	UNP Q9E006
D	1237	ILE	-	expression tag	UNP Q9E006
D	1238	PHE	-	expression tag	UNP Q9E006
D	1239	GLU	-	expression tag	UNP Q9E006
D	1240	LEU	-	expression tag	UNP Q9E006
D	1241	GLU	-	expression tag	UNP Q9E006
D	1242	LYS	-	expression tag	UNP Q9E006
D	1243	LYS	-	expression tag	UNP Q9E006
D	1244	THR	-	expression tag	UNP Q9E006
D	1245	GLU	-	expression tag	UNP Q9E006
D	1246	THR	-	expression tag	UNP Q9E006
D	1247	ALA	-	expression tag	UNP Q9E006

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1248	ALA	-	expression tag	UNP Q9E006
D	1249	GLY	-	expression tag	UNP Q9E006
D	1250	GLY	-	expression tag	UNP Q9E006
D	1251	GLY	-	expression tag	UNP Q9E006
D	1252	SER	-	expression tag	UNP Q9E006
D	1253	HIS	-	expression tag	UNP Q9E006
D	1254	HIS	-	expression tag	UNP Q9E006
D	1255	HIS	-	expression tag	UNP Q9E006
D	1256	HIS	-	expression tag	UNP Q9E006
D	1257	HIS	-	expression tag	UNP Q9E006
D	1258	HIS	-	expression tag	UNP Q9E006
D	1259	HIS	-	expression tag	UNP Q9E006
D	1260	HIS	-	expression tag	UNP Q9E006
F	1096	LEU	SER	engineered mutation	UNP Q9E006
F	1139	GLY	-	expression tag	UNP Q9E006
F	1140	SER	-	expression tag	UNP Q9E006
F	1141	GLY	-	expression tag	UNP Q9E006
F	1142	SER	-	expression tag	UNP Q9E006
F	1143	ALA	-	expression tag	UNP Q9E006
F	1144	LEU	-	expression tag	UNP Q9E006
F	1145	PRO	-	expression tag	UNP Q9E006
F	1146	GLY	-	expression tag	UNP Q9E006
F	1147	ASN	-	expression tag	UNP Q9E006
F	1148	PRO	-	expression tag	UNP Q9E006
F	1149	ASP	-	expression tag	UNP Q9E006
F	1150	HIS	-	expression tag	UNP Q9E006
F	1151	ARG	-	expression tag	UNP Q9E006
F	1152	GLU	-	expression tag	UNP Q9E006
F	1153	MET	-	expression tag	UNP Q9E006
F	1154	GLY	-	expression tag	UNP Q9E006
F	1155	GLU	-	expression tag	UNP Q9E006
F	1156	THR	-	expression tag	UNP Q9E006
F	1157	LEU	-	expression tag	UNP Q9E006
F	1158	PRO	-	expression tag	UNP Q9E006
F	1159	GLU	-	expression tag	UNP Q9E006
F	1160	GLU	-	expression tag	UNP Q9E006
F	1161	VAL	-	expression tag	UNP Q9E006
F	1162	GLY	-	expression tag	UNP Q9E006
F	1163	GLU	-	expression tag	UNP Q9E006
F	1164	TYR	-	expression tag	UNP Q9E006
F	1165	ARG	-	expression tag	UNP Q9E006
F	1166	GLN	-	expression tag	UNP Q9E006

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1167	PRO	-	expression tag	UNP Q9E006
F	1168	SER	-	expression tag	UNP Q9E006
F	1169	GLY	-	expression tag	UNP Q9E006
F	1170	GLY	-	expression tag	UNP Q9E006
F	1171	SER	-	expression tag	UNP Q9E006
F	1172	VAL	-	expression tag	UNP Q9E006
F	1173	PRO	-	expression tag	UNP Q9E006
F	1174	VAL	-	expression tag	UNP Q9E006
F	1175	SER	-	expression tag	UNP Q9E006
F	1176	PRO	-	expression tag	UNP Q9E006
F	1177	GLY	-	expression tag	UNP Q9E006
F	1178	PRO	-	expression tag	UNP Q9E006
F	1179	PRO	-	expression tag	UNP Q9E006
F	1180	SER	-	expression tag	UNP Q9E006
F	1181	GLY	-	expression tag	UNP Q9E006
F	1182	LEU	-	expression tag	UNP Q9E006
F	1183	GLU	-	expression tag	UNP Q9E006
F	1184	PRO	-	expression tag	UNP Q9E006
F	1185	THR	-	expression tag	UNP Q9E006
F	1186	SER	-	expression tag	UNP Q9E006
F	1187	SER	-	expression tag	UNP Q9E006
F	1188	SER	-	expression tag	UNP Q9E006
F	1189	PRO	-	expression tag	UNP Q9E006
F	1190	TYR	-	expression tag	UNP Q9E006
F	1191	GLY	-	expression tag	UNP Q9E006
F	1192	GLY	-	expression tag	UNP Q9E006
F	1193	GLY	-	expression tag	UNP Q9E006
F	1194	SER	-	expression tag	UNP Q9E006
F	1195	PHE	-	expression tag	UNP Q9E006
F	1196	ASN	-	expression tag	UNP Q9E006
F	1197	SER	-	expression tag	UNP Q9E006
F	1198	SER	-	expression tag	UNP Q9E006
F	1199	ILE	-	expression tag	UNP Q9E006
F	1200	ASN	-	expression tag	UNP Q9E006
F	1201	ASN	-	expression tag	UNP Q9E006
F	1202	ILE	-	expression tag	UNP Q9E006
F	1203	HIS	-	expression tag	UNP Q9E006
F	1204	GLU	-	expression tag	UNP Q9E006
F	1205	MET	-	expression tag	UNP Q9E006
F	1206	GLU	-	expression tag	UNP Q9E006
F	1207	ILE	-	expression tag	UNP Q9E006
F	1208	GLN	-	expression tag	UNP Q9E006

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1209	LEU	-	expression tag	UNP Q9E006
F	1210	LYS	-	expression tag	UNP Q9E006
F	1211	ASP	-	expression tag	UNP Q9E006
F	1212	ALA	-	expression tag	UNP Q9E006
F	1213	LEU	-	expression tag	UNP Q9E006
F	1214	GLU	-	expression tag	UNP Q9E006
F	1215	LYS	-	expression tag	UNP Q9E006
F	1216	ASN	-	expression tag	UNP Q9E006
F	1217	GLN	-	expression tag	UNP Q9E006
F	1218	GLN	-	expression tag	UNP Q9E006
F	1219	TRP	-	expression tag	UNP Q9E006
F	1220	LEU	-	expression tag	UNP Q9E006
F	1221	VAL	-	expression tag	UNP Q9E006
F	1222	TYR	-	expression tag	UNP Q9E006
F	1223	ASP	-	expression tag	UNP Q9E006
F	1224	GLN	-	expression tag	UNP Q9E006
F	1225	GLN	-	expression tag	UNP Q9E006
F	1226	ARG	-	expression tag	UNP Q9E006
F	1227	GLU	-	expression tag	UNP Q9E006
F	1228	VAL	-	expression tag	UNP Q9E006
F	1229	TYR	-	expression tag	UNP Q9E006
F	1230	VAL	-	expression tag	UNP Q9E006
F	1231	LYS	-	expression tag	UNP Q9E006
F	1232	GLY	-	expression tag	UNP Q9E006
F	1233	LEU	-	expression tag	UNP Q9E006
F	1234	LEU	-	expression tag	UNP Q9E006
F	1235	ALA	-	expression tag	UNP Q9E006
F	1236	LYS	-	expression tag	UNP Q9E006
F	1237	ILE	-	expression tag	UNP Q9E006
F	1238	PHE	-	expression tag	UNP Q9E006
F	1239	GLU	-	expression tag	UNP Q9E006
F	1240	LEU	-	expression tag	UNP Q9E006
F	1241	GLU	-	expression tag	UNP Q9E006
F	1242	LYS	-	expression tag	UNP Q9E006
F	1243	LYS	-	expression tag	UNP Q9E006
F	1244	THR	-	expression tag	UNP Q9E006
F	1245	GLU	-	expression tag	UNP Q9E006
F	1246	THR	-	expression tag	UNP Q9E006
F	1247	ALA	-	expression tag	UNP Q9E006
F	1248	ALA	-	expression tag	UNP Q9E006
F	1249	GLY	-	expression tag	UNP Q9E006
F	1250	GLY	-	expression tag	UNP Q9E006

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1251	GLY	-	expression tag	UNP Q9E006
F	1252	SER	-	expression tag	UNP Q9E006
F	1253	HIS	-	expression tag	UNP Q9E006
F	1254	HIS	-	expression tag	UNP Q9E006
F	1255	HIS	-	expression tag	UNP Q9E006
F	1256	HIS	-	expression tag	UNP Q9E006
F	1257	HIS	-	expression tag	UNP Q9E006
F	1258	HIS	-	expression tag	UNP Q9E006
F	1259	HIS	-	expression tag	UNP Q9E006
F	1260	HIS	-	expression tag	UNP Q9E006
H	1096	LEU	SER	engineered mutation	UNP Q9E006
H	1139	GLY	-	expression tag	UNP Q9E006
H	1140	SER	-	expression tag	UNP Q9E006
H	1141	GLY	-	expression tag	UNP Q9E006
H	1142	SER	-	expression tag	UNP Q9E006
H	1143	ALA	-	expression tag	UNP Q9E006
H	1144	LEU	-	expression tag	UNP Q9E006
H	1145	PRO	-	expression tag	UNP Q9E006
H	1146	GLY	-	expression tag	UNP Q9E006
H	1147	ASN	-	expression tag	UNP Q9E006
H	1148	PRO	-	expression tag	UNP Q9E006
H	1149	ASP	-	expression tag	UNP Q9E006
H	1150	HIS	-	expression tag	UNP Q9E006
H	1151	ARG	-	expression tag	UNP Q9E006
H	1152	GLU	-	expression tag	UNP Q9E006
H	1153	MET	-	expression tag	UNP Q9E006
H	1154	GLY	-	expression tag	UNP Q9E006
H	1155	GLU	-	expression tag	UNP Q9E006
H	1156	THR	-	expression tag	UNP Q9E006
H	1157	LEU	-	expression tag	UNP Q9E006
H	1158	PRO	-	expression tag	UNP Q9E006
H	1159	GLU	-	expression tag	UNP Q9E006
H	1160	GLU	-	expression tag	UNP Q9E006
H	1161	VAL	-	expression tag	UNP Q9E006
H	1162	GLY	-	expression tag	UNP Q9E006
H	1163	GLU	-	expression tag	UNP Q9E006
H	1164	TYR	-	expression tag	UNP Q9E006
H	1165	ARG	-	expression tag	UNP Q9E006
H	1166	GLN	-	expression tag	UNP Q9E006
H	1167	PRO	-	expression tag	UNP Q9E006
H	1168	SER	-	expression tag	UNP Q9E006
H	1169	GLY	-	expression tag	UNP Q9E006

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Chain	Residue	Modelled	Actual	Comment	Reference
H	1170	GLY	-	expression tag	UNP Q9E006
H	1171	SER	-	expression tag	UNP Q9E006
H	1172	VAL	-	expression tag	UNP Q9E006
H	1173	PRO	-	expression tag	UNP Q9E006
H	1174	VAL	-	expression tag	UNP Q9E006
H	1175	SER	-	expression tag	UNP Q9E006
H	1176	PRO	-	expression tag	UNP Q9E006
H	1177	GLY	-	expression tag	UNP Q9E006
H	1178	PRO	-	expression tag	UNP Q9E006
H	1179	PRO	-	expression tag	UNP Q9E006
H	1180	SER	-	expression tag	UNP Q9E006
H	1181	GLY	-	expression tag	UNP Q9E006
H	1182	LEU	-	expression tag	UNP Q9E006
H	1183	GLU	-	expression tag	UNP Q9E006
H	1184	PRO	-	expression tag	UNP Q9E006
H	1185	THR	-	expression tag	UNP Q9E006
H	1186	SER	-	expression tag	UNP Q9E006
H	1187	SER	-	expression tag	UNP Q9E006
H	1188	SER	-	expression tag	UNP Q9E006
H	1189	PRO	-	expression tag	UNP Q9E006
H	1190	TYR	-	expression tag	UNP Q9E006
H	1191	GLY	-	expression tag	UNP Q9E006
H	1192	GLY	-	expression tag	UNP Q9E006
H	1193	GLY	-	expression tag	UNP Q9E006
H	1194	SER	-	expression tag	UNP Q9E006
H	1195	PHE	-	expression tag	UNP Q9E006
H	1196	ASN	-	expression tag	UNP Q9E006
H	1197	SER	-	expression tag	UNP Q9E006
H	1198	SER	-	expression tag	UNP Q9E006
H	1199	ILE	-	expression tag	UNP Q9E006
H	1200	ASN	-	expression tag	UNP Q9E006
H	1201	ASN	-	expression tag	UNP Q9E006
H	1202	ILE	-	expression tag	UNP Q9E006
H	1203	HIS	-	expression tag	UNP Q9E006
H	1204	GLU	-	expression tag	UNP Q9E006
H	1205	MET	-	expression tag	UNP Q9E006
H	1206	GLU	-	expression tag	UNP Q9E006
H	1207	ILE	-	expression tag	UNP Q9E006
H	1208	GLN	-	expression tag	UNP Q9E006
H	1209	LEU	-	expression tag	UNP Q9E006
H	1210	LYS	-	expression tag	UNP Q9E006
H	1211	ASP	-	expression tag	UNP Q9E006

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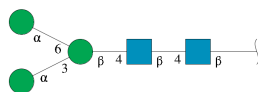
Chain	Residue	Modelled	Actual	Comment	Reference
H	1212	ALA	-	expression tag	UNP Q9E006
H	1213	LEU	-	expression tag	UNP Q9E006
H	1214	GLU	-	expression tag	UNP Q9E006
H	1215	LYS	-	expression tag	UNP Q9E006
H	1216	ASN	-	expression tag	UNP Q9E006
H	1217	GLN	-	expression tag	UNP Q9E006
H	1218	GLN	-	expression tag	UNP Q9E006
H	1219	TRP	-	expression tag	UNP Q9E006
H	1220	LEU	-	expression tag	UNP Q9E006
H	1221	VAL	-	expression tag	UNP Q9E006
H	1222	TYR	-	expression tag	UNP Q9E006
H	1223	ASP	-	expression tag	UNP Q9E006
H	1224	GLN	-	expression tag	UNP Q9E006
H	1225	GLN	-	expression tag	UNP Q9E006
H	1226	ARG	-	expression tag	UNP Q9E006
H	1227	GLU	-	expression tag	UNP Q9E006
H	1228	VAL	-	expression tag	UNP Q9E006
H	1229	TYR	-	expression tag	UNP Q9E006
H	1230	VAL	-	expression tag	UNP Q9E006
H	1231	LYS	-	expression tag	UNP Q9E006
H	1232	GLY	-	expression tag	UNP Q9E006
H	1233	LEU	-	expression tag	UNP Q9E006
H	1234	LEU	-	expression tag	UNP Q9E006
H	1235	ALA	-	expression tag	UNP Q9E006
H	1236	LYS	-	expression tag	UNP Q9E006
H	1237	ILE	-	expression tag	UNP Q9E006
H	1238	PHE	-	expression tag	UNP Q9E006
H	1239	GLU	-	expression tag	UNP Q9E006
H	1240	LEU	-	expression tag	UNP Q9E006
H	1241	GLU	-	expression tag	UNP Q9E006
H	1242	LYS	-	expression tag	UNP Q9E006
H	1243	LYS	-	expression tag	UNP Q9E006
H	1244	THR	-	expression tag	UNP Q9E006
H	1245	GLU	-	expression tag	UNP Q9E006
H	1246	THR	-	expression tag	UNP Q9E006
H	1247	ALA	-	expression tag	UNP Q9E006
H	1248	ALA	-	expression tag	UNP Q9E006
H	1249	GLY	-	expression tag	UNP Q9E006
H	1250	GLY	-	expression tag	UNP Q9E006
H	1251	GLY	-	expression tag	UNP Q9E006
H	1252	SER	-	expression tag	UNP Q9E006
H	1253	HIS	-	expression tag	UNP Q9E006

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Chain	Residue	Modelled	Actual	Comment	Reference
H	1254	HIS	-	expression tag	UNP Q9E006
H	1255	HIS	-	expression tag	UNP Q9E006
H	1256	HIS	-	expression tag	UNP Q9E006
H	1257	HIS	-	expression tag	UNP Q9E006
H	1258	HIS	-	expression tag	UNP Q9E006
H	1259	HIS	-	expression tag	UNP Q9E006
H	1260	HIS	-	expression tag	UNP Q9E006

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



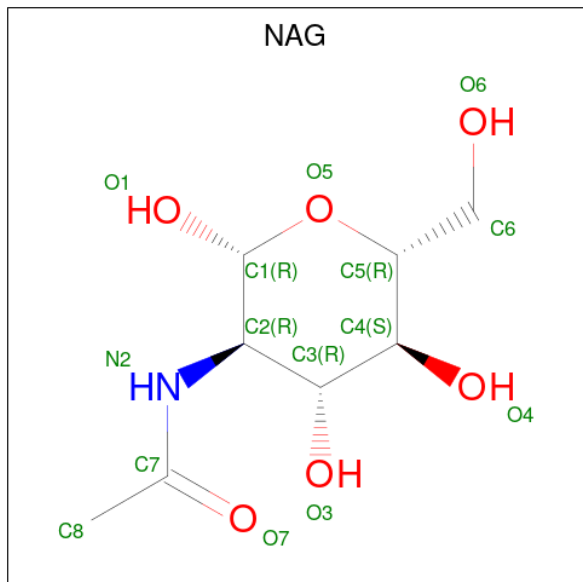
Mol	Chain	Residues	Atoms				AltConf	Trace
5	Q	5	Total	C	N	O	0	0
			61	34	2	25		
5	S	5	Total	C	N	O	0	0
			61	34	2	25		
5	U	5	Total	C	N	O	0	0
			61	34	2	25		
5	W	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	R	2	Total	C	N	O	0	0
			28	16	2	10		
6	T	2	Total	C	N	O	0	0
			28	16	2	10		
6	V	2	Total	C	N	O	0	0
			28	16	2	10		
6	X	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

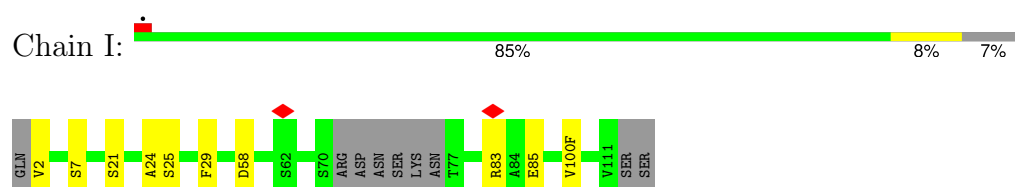


Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	E	1	Total	C	N	O	0
			14	8	1	5	
7	G	1	Total	C	N	O	0
			14	8	1	5	

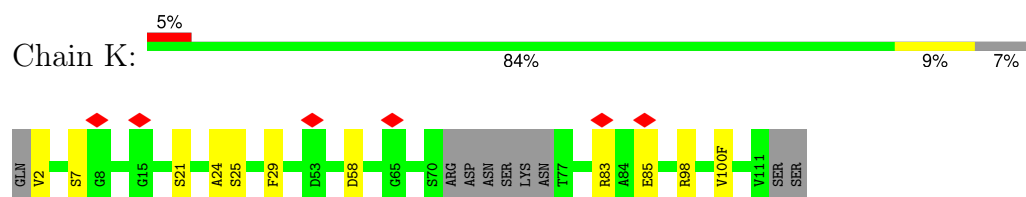
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

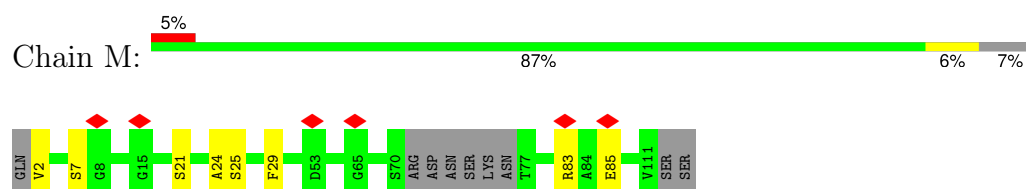
- Molecule 1: ADI-65534 variable heavy chain



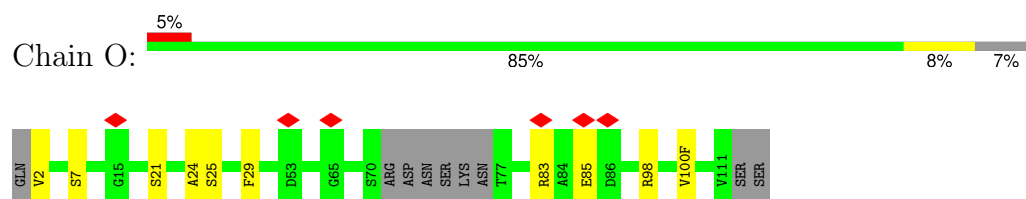
- Molecule 1: ADI-65534 variable heavy chain



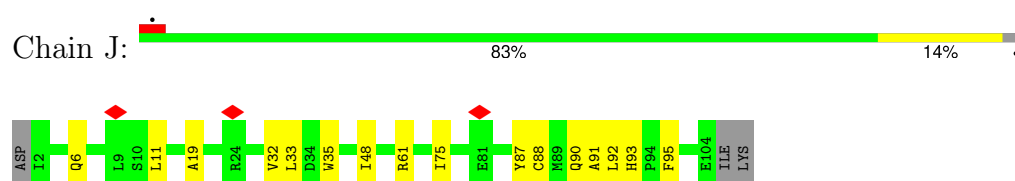
- Molecule 1: ADI-65534 variable heavy chain



- Molecule 1: ADI-65534 variable heavy chain

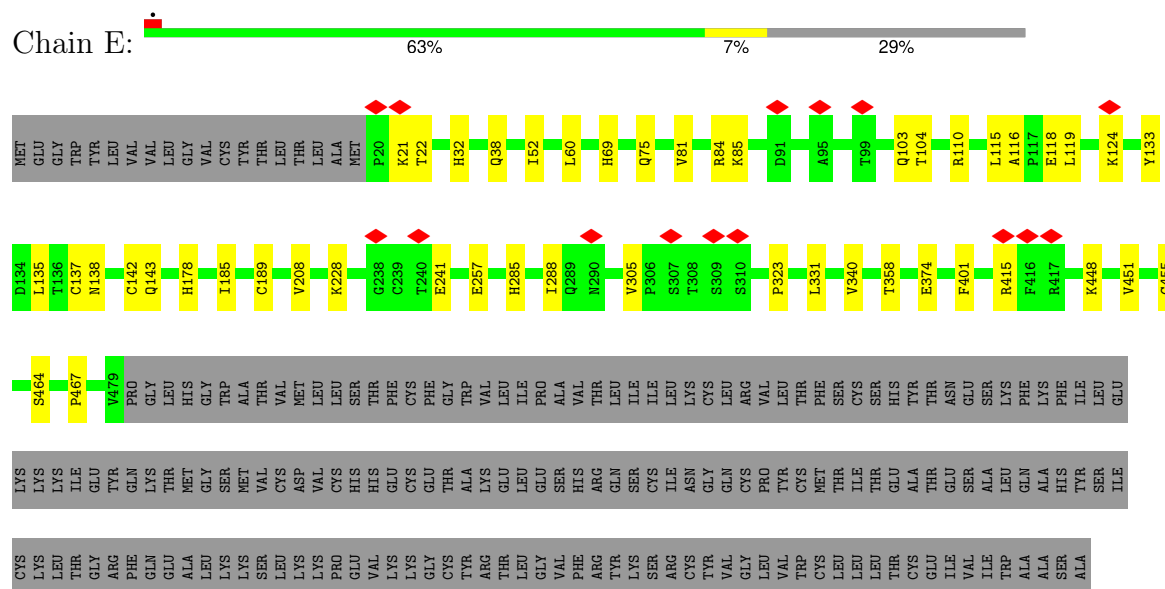


- Molecule 2: ADI-65534 variable light chain

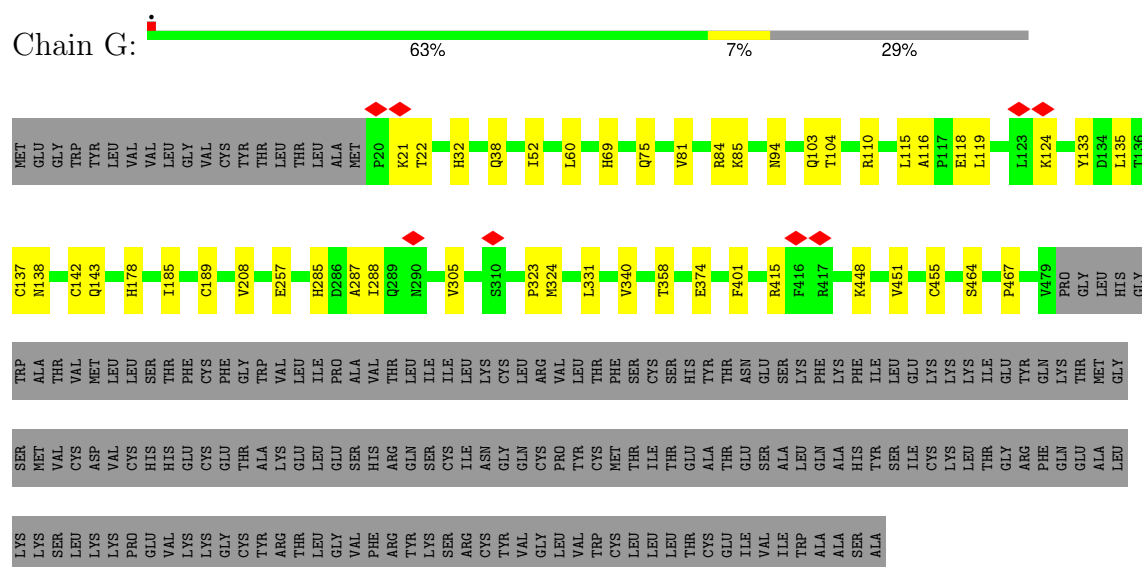


- MET
 GLU
 GLY
 TRP
 TYR
 LEU
 VAL
 VAL
 VAL
 LEU
 GLY
 VAL
 CYS
 TYR
 THR
 THR
 THR
 LEU
 ALA
 MET
- P20
 K21
 T22
 H32
 I52
 L60
 H69
 Q75
 V81
 R84
 K86
 N94
 Q103
 T104
 R110
 L115
 A116
 L119
 L123
 K124
 K125
 Y133
 D134
 L136
 T136
 C137
 N138

- Molecule 3: Glycoprotein N

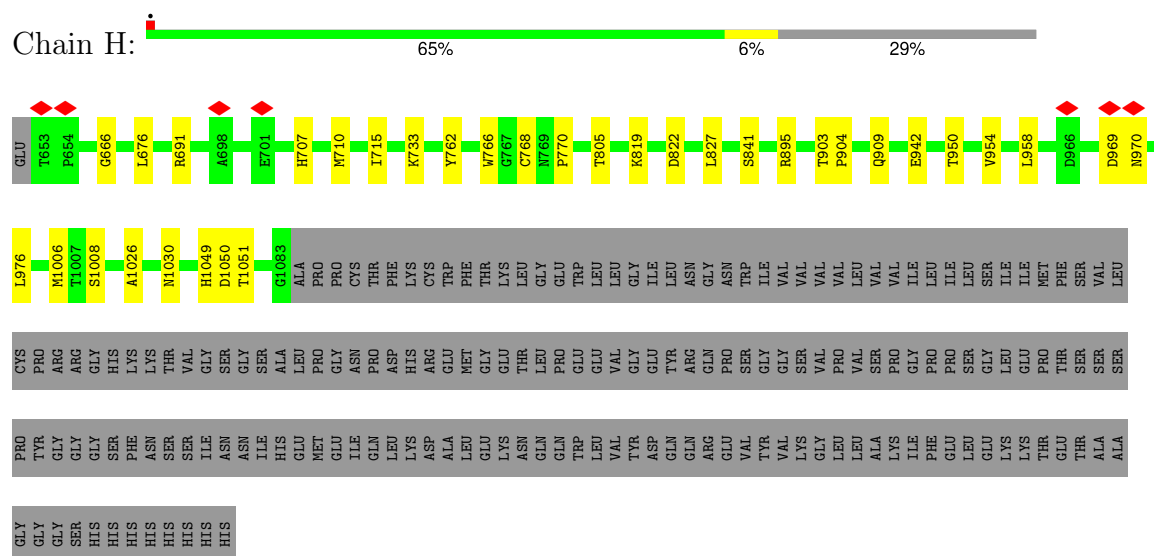


- Molecule 3: Glycoprotein N

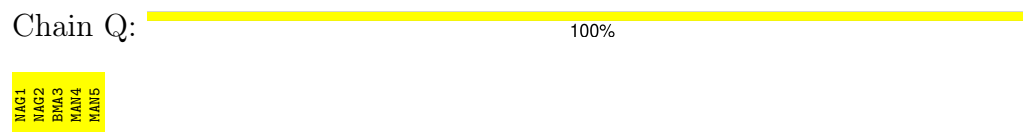


- Molecule 4: Glycoprotein C

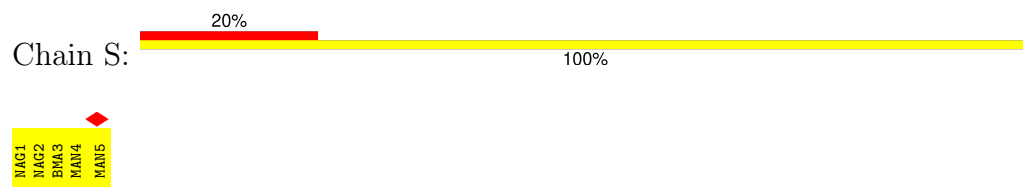
- Molecule 4: Glycoprotein C



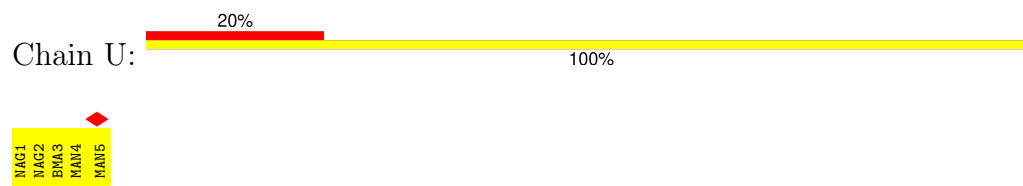
- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12483	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	17.550	Depositor
Minimum map value	-0.072	Depositor
Average map value	0.047	Depositor
Map value standard deviation	0.568	Depositor
Recommended contour level	3.8	Depositor
Map size (Å)	419.328, 419.328, 331.13602	wwPDB
Map dimensions	504, 504, 398	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MAN, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	I	0.19	0/940	0.39	0/1275
1	K	0.20	0/940	0.40	0/1275
1	M	0.20	0/940	0.40	0/1275
1	O	0.20	0/940	0.40	0/1275
2	J	0.15	0/841	0.35	0/1144
2	L	0.15	0/841	0.36	0/1144
2	N	0.14	0/841	0.37	0/1144
2	P	0.14	0/841	0.36	0/1144
3	A	0.16	0/3593	0.37	0/4886
3	C	0.15	0/3593	0.37	0/4886
3	E	0.15	0/3593	0.36	0/4886
3	G	0.14	0/3593	0.36	0/4886
4	B	0.13	0/3375	0.34	0/4576
4	D	0.14	0/3375	0.34	0/4576
4	F	0.14	0/3375	0.34	0/4576
4	H	0.13	0/3375	0.33	0/4576
All	All	0.15	0/34996	0.36	0/47524

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	917	0	887	7	0
1	K	917	0	887	9	0
1	M	917	0	887	5	0
1	O	917	0	887	7	0
2	J	820	0	797	10	0
2	L	820	0	797	10	0
2	N	820	0	797	7	0
2	P	820	0	797	9	0
3	A	3523	0	3518	33	0
3	C	3523	0	3518	29	0
3	E	3523	0	3518	31	0
3	G	3523	0	3518	31	0
4	B	3296	0	3154	17	0
4	D	3296	0	3154	20	0
4	F	3296	0	3154	20	0
4	H	3296	0	3154	23	0
5	Q	61	0	52	0	0
5	S	61	0	52	0	0
5	U	61	0	52	0	0
5	W	61	0	52	0	0
6	R	28	0	25	0	0
6	T	28	0	25	0	0
6	V	28	0	25	0	0
6	X	28	0	25	0	0
7	A	14	0	13	0	0
7	C	14	0	13	0	0
7	E	14	0	13	0	0
7	G	14	0	13	0	0
All	All	34636	0	33784	244	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (244) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:32:VAL:HG11	2:P:92:LEU:HG	1.64	0.80
2:J:32:VAL:HG11	2:J:92:LEU:HG	1.62	0.80
2:L:32:VAL:HG11	2:L:92:LEU:HG	1.62	0.79
3:E:228:LYS:HE3	3:E:241:GLU:HG3	1.72	0.72
3:C:75:GLN:HG2	3:C:110:ARG:HB2	1.76	0.67
3:A:75:GLN:HG2	3:A:110:ARG:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:75:GLN:HG2	3:G:110:ARG:HB2	1.76	0.66
3:E:75:GLN:HG2	3:E:110:ARG:HB2	1.76	0.66
4:D:691:ARG:NH2	4:D:1050:ASP:OD1	2.30	0.65
4:B:691:ARG:NH2	4:B:1050:ASP:OD1	2.31	0.64
4:H:691:ARG:NH2	4:H:1050:ASP:OD1	2.30	0.64
4:F:691:ARG:NH2	4:F:1050:ASP:OD1	2.31	0.63
3:E:118:GLU:HB2	3:E:124:LYS:HE2	1.84	0.60
4:H:707:HIS:HD2	4:H:1006:MET:HE3	1.66	0.60
2:L:35:TRP:HB2	2:L:48:ILE:HB	1.83	0.60
2:N:35:TRP:HB2	2:N:48:ILE:HB	1.83	0.60
2:J:35:TRP:HB2	2:J:48:ILE:HB	1.83	0.59
2:P:35:TRP:HB2	2:P:48:ILE:HB	1.83	0.58
4:F:676:LEU:HB3	4:F:958:LEU:HB3	1.85	0.58
3:G:118:GLU:HB2	3:G:124:LYS:HE2	1.86	0.58
4:D:676:LEU:HB3	4:D:958:LEU:HB3	1.85	0.57
4:H:676:LEU:HB3	4:H:958:LEU:HB3	1.85	0.57
3:G:288:ILE:HG12	3:G:323:PRO:O	2.04	0.57
4:B:676:LEU:HB3	4:B:958:LEU:HB3	1.86	0.57
3:E:288:ILE:HG12	3:E:323:PRO:O	2.04	0.57
3:A:288:ILE:HG12	3:A:323:PRO:O	2.04	0.56
3:C:288:ILE:HG12	3:C:323:PRO:O	2.04	0.56
3:E:115:LEU:HB3	3:E:119:LEU:HD12	1.88	0.56
3:C:21:LYS:HG3	3:C:22:THR:H	1.71	0.56
4:F:819:LYS:HD3	4:F:827:LEU:HD13	1.88	0.56
4:H:707:HIS:CD2	4:H:1006:MET:HE3	2.40	0.56
3:A:32:HIS:HE2	3:A:178:HIS:HA	1.71	0.55
3:A:21:LYS:HG3	3:A:22:THR:H	1.71	0.55
3:G:115:LEU:HB3	3:G:119:LEU:HD12	1.88	0.55
4:H:819:LYS:HD3	4:H:827:LEU:HD13	1.89	0.55
2:N:92:LEU:HG	2:N:93:HIS:H	1.72	0.55
4:B:819:LYS:HD3	4:B:827:LEU:HD13	1.88	0.55
4:D:969:ASP:OD1	4:D:970:ASN:N	2.40	0.55
4:H:1026:ALA:H	4:H:1030:ASN:HD21	1.55	0.55
3:C:32:HIS:HE2	3:C:178:HIS:HA	1.71	0.55
3:C:115:LEU:HB3	3:C:119:LEU:HD12	1.89	0.55
4:D:1026:ALA:H	4:D:1030:ASN:HD21	1.55	0.55
3:G:21:LYS:HG3	3:G:22:THR:H	1.71	0.55
3:G:32:HIS:HE2	3:G:178:HIS:HA	1.71	0.55
4:D:819:LYS:HD3	4:D:827:LEU:HD13	1.88	0.54
4:F:969:ASP:OD1	4:F:970:ASN:N	2.40	0.54
1:O:98:ARG:HH21	4:H:762:TYR:HE2	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:115:LEU:HB3	3:A:119:LEU:HD12	1.89	0.54
4:B:969:ASP:OD1	4:B:970:ASN:N	2.40	0.54
3:E:21:LYS:HG3	3:E:22:THR:H	1.72	0.54
4:B:1026:ALA:H	4:B:1030:ASN:HD21	1.56	0.54
3:E:32:HIS:HE2	3:E:178:HIS:HA	1.71	0.54
2:J:33:LEU:HD11	2:J:88:CYS:HB2	1.90	0.53
2:P:33:LEU:HD11	2:P:88:CYS:HB2	1.90	0.53
1:K:100(F):VAL:HA	3:C:94:ASN:HD22	1.74	0.53
3:A:331:LEU:HD23	3:A:358:THR:HG22	1.90	0.53
3:G:331:LEU:HD23	3:G:358:THR:HG22	1.91	0.53
1:K:98:ARG:HH21	4:D:762:TYR:HE2	1.57	0.52
2:L:33:LEU:HD11	2:L:88:CYS:HB2	1.90	0.52
1:I:2:VAL:HA	1:I:25:SER:O	2.10	0.52
1:O:2:VAL:HA	1:O:25:SER:O	2.10	0.52
1:M:2:VAL:HA	1:M:25:SER:O	2.10	0.52
3:E:331:LEU:HD23	3:E:358:THR:HG22	1.91	0.52
3:C:331:LEU:HD23	3:C:358:THR:HG22	1.91	0.51
4:H:805:THR:HG22	4:H:822:ASP:HB3	1.93	0.51
4:H:969:ASP:OD1	4:H:970:ASN:N	2.40	0.51
2:N:33:LEU:HD11	2:N:88:CYS:HB2	1.91	0.51
1:O:7:SER:OG	1:O:21:SER:OG	2.29	0.51
1:O:100(F):VAL:HA	3:G:94:ASN:HD22	1.76	0.51
1:I:7:SER:OG	1:I:21:SER:OG	2.29	0.50
4:B:805:THR:HG22	4:B:822:ASP:HB3	1.93	0.50
4:F:805:THR:HG22	4:F:822:ASP:HB3	1.92	0.50
3:A:467:PRO:HB2	3:C:448:LYS:HG3	1.94	0.50
4:D:805:THR:HG22	4:D:822:ASP:HB3	1.92	0.50
1:M:7:SER:OG	1:M:21:SER:OG	2.29	0.50
1:K:2:VAL:HA	1:K:25:SER:O	2.10	0.50
4:F:1026:ALA:H	4:F:1030:ASN:HD21	1.60	0.50
1:I:58:ASP:HB3	2:J:93:HIS:CE1	2.47	0.49
3:A:135:LEU:HB3	3:A:137:CYS:SG	2.52	0.49
3:E:135:LEU:HB3	3:E:137:CYS:SG	2.52	0.49
1:K:7:SER:OG	1:K:21:SER:OG	2.29	0.49
1:K:58:ASP:HB3	2:L:93:HIS:CE1	2.47	0.49
3:C:467:PRO:HB2	3:E:448:LYS:HG3	1.94	0.49
3:G:143:GLN:OE1	3:G:288:ILE:HD12	2.13	0.49
3:A:189:CYS:HB2	3:A:374:GLU:HB2	1.94	0.49
3:A:448:LYS:HG3	3:G:467:PRO:HB2	1.95	0.49
3:E:143:GLN:OE1	3:E:288:ILE:HD12	2.13	0.49
3:E:228:LYS:HZ2	3:E:241:GLU:HA	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:467:PRO:HB2	3:G:448:LYS:HG3	1.95	0.48
2:J:11:LEU:HD21	2:J:19:ALA:HB1	1.96	0.48
2:P:11:LEU:HD21	2:P:19:ALA:HB1	1.96	0.48
4:B:691:ARG:HH11	4:B:1008:SER:HB2	1.78	0.48
3:G:135:LEU:HB3	3:G:137:CYS:SG	2.52	0.48
3:E:52:ILE:HD13	3:E:142:CYS:HB2	1.95	0.48
3:E:285:HIS:HB3	4:F:733:LYS:HZ1	1.78	0.48
3:C:135:LEU:HB3	3:C:137:CYS:SG	2.52	0.48
3:C:143:GLN:OE1	3:C:288:ILE:HD12	2.13	0.48
3:A:143:GLN:OE1	3:A:288:ILE:HD12	2.13	0.48
4:F:841:SER:HB2	4:F:950:THR:HG23	1.96	0.48
3:E:189:CYS:HB2	3:E:374:GLU:HB2	1.95	0.48
3:C:52:ILE:HD13	3:C:142:CYS:HB2	1.95	0.48
3:G:52:ILE:HD13	3:G:142:CYS:HB2	1.95	0.48
2:L:11:LEU:HD21	2:L:19:ALA:HB1	1.96	0.47
3:G:285:HIS:HB3	4:H:733:LYS:HZ1	1.78	0.47
2:N:11:LEU:HD21	2:N:19:ALA:HB1	1.96	0.47
4:B:895:ARG:HD3	4:B:909:GLN:HE22	1.78	0.47
3:C:189:CYS:HB2	3:C:374:GLU:HB2	1.95	0.47
4:D:841:SER:HB2	4:D:950:THR:HG23	1.95	0.47
4:F:895:ARG:HD3	4:F:909:GLN:HE22	1.79	0.47
4:H:766:TRP:CZ2	4:H:768:CYS:HB3	2.49	0.47
4:H:895:ARG:HD3	4:H:909:GLN:HE22	1.79	0.47
3:G:189:CYS:HB2	3:G:374:GLU:HB2	1.96	0.47
2:N:6:GLN:HE22	2:N:87:TYR:HA	1.79	0.47
4:B:766:TRP:HH2	4:B:904:PRO:HG3	1.79	0.47
1:O:24:ALA:HB3	1:O:29:PHE:HE1	1.79	0.47
3:C:464:SER:HB2	3:E:455:CYS:HB2	1.96	0.47
4:D:766:TRP:HH2	4:D:904:PRO:HG3	1.80	0.47
1:K:24:ALA:HB3	1:K:29:PHE:HE1	1.79	0.47
1:M:24:ALA:HB3	1:M:29:PHE:HE1	1.79	0.47
2:P:6:GLN:HE22	2:P:87:TYR:HA	1.79	0.47
3:A:455:CYS:HB2	3:G:464:SER:HB2	1.96	0.47
4:B:841:SER:HB2	4:B:950:THR:HG23	1.96	0.47
3:E:464:SER:HB2	3:G:455:CYS:HB2	1.96	0.47
4:F:691:ARG:HH11	4:F:1008:SER:HB2	1.80	0.47
4:F:766:TRP:HH2	4:F:904:PRO:HG3	1.80	0.47
4:H:691:ARG:HH11	4:H:1008:SER:HB2	1.80	0.47
2:L:6:GLN:HE22	2:L:87:TYR:HA	1.79	0.47
3:C:285:HIS:HB3	4:D:733:LYS:HZ1	1.80	0.47
4:D:895:ARG:HD3	4:D:909:GLN:HE22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:766:TRP:CZ2	4:F:768:CYS:HB3	2.50	0.47
3:A:451:VAL:HG11	3:G:467:PRO:HA	1.96	0.46
4:H:841:SER:HB2	4:H:950:THR:HG23	1.96	0.46
3:A:464:SER:HB2	3:C:455:CYS:HB2	1.96	0.46
3:C:467:PRO:HA	3:E:451:VAL:HG11	1.96	0.46
4:B:766:TRP:CZ2	4:B:768:CYS:HB3	2.50	0.46
1:I:24:ALA:HB3	1:I:29:PHE:HE1	1.80	0.46
3:C:81:VAL:HG22	3:C:104:THR:HG22	1.97	0.46
4:H:766:TRP:HH2	4:H:904:PRO:HG3	1.80	0.46
4:D:766:TRP:CZ2	4:D:768:CYS:HB3	2.50	0.46
3:E:467:PRO:HA	3:G:451:VAL:HG11	1.97	0.46
3:A:52:ILE:HD13	3:A:142:CYS:HB2	1.98	0.46
3:A:467:PRO:HA	3:C:451:VAL:HG11	1.96	0.46
3:E:401:PHE:HB3	3:E:415:ARG:HG2	1.98	0.46
3:G:81:VAL:HG22	3:G:104:THR:HG22	1.97	0.46
2:J:32:VAL:HG12	2:J:91:ALA:H	1.81	0.45
2:J:6:GLN:HE22	2:J:87:TYR:HA	1.79	0.45
2:L:90:GLN:O	2:L:95:PHE:HA	2.16	0.45
3:A:81:VAL:HG22	3:A:104:THR:HG22	1.98	0.45
4:B:770:PRO:HB3	4:B:903:THR:HG22	1.99	0.45
3:E:81:VAL:HG22	3:E:104:THR:HG22	1.97	0.45
4:D:691:ARG:HH11	4:D:1008:SER:HB2	1.81	0.45
3:G:401:PHE:HB3	3:G:415:ARG:HG2	1.98	0.45
2:J:32:VAL:HG13	2:J:91:ALA:HB3	1.99	0.45
3:A:401:PHE:HB3	3:A:415:ARG:HG2	1.98	0.45
2:P:32:VAL:HG12	2:P:91:ALA:H	1.82	0.44
2:L:32:VAL:HG12	2:L:91:ALA:H	1.81	0.44
3:C:401:PHE:HB3	3:C:415:ARG:HG2	1.98	0.44
4:B:666:GLY:HA2	4:B:1051:THR:HG22	1.99	0.44
3:E:60:LEU:HD11	3:E:133:TYR:HD1	1.83	0.44
4:H:770:PRO:HB3	4:H:903:THR:HG22	1.99	0.44
4:D:770:PRO:HB3	4:D:903:THR:HG22	1.99	0.44
4:F:666:GLY:HA2	4:F:1051:THR:HG22	1.99	0.44
2:P:32:VAL:HG13	2:P:91:ALA:HB3	1.99	0.43
4:F:770:PRO:HB3	4:F:903:THR:HG22	1.99	0.43
2:J:90:GLN:O	2:J:95:PHE:HA	2.17	0.43
4:D:666:GLY:HA2	4:D:1051:THR:HG22	1.99	0.43
4:F:715:ILE:O	4:F:942:GLU:HA	2.18	0.43
1:K:100(F):VAL:HB	3:C:94:ASN:HB3	2.00	0.43
2:L:32:VAL:HG13	2:L:91:ALA:HB3	1.99	0.43
4:H:715:ILE:O	4:H:942:GLU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:83:ARG:HB3	1:I:85:GLU:OE1	2.19	0.43
4:H:666:GLY:HA2	4:H:1051:THR:HG22	1.99	0.43
4:F:976:LEU:HD11	4:F:1049:HIS:HB3	2.00	0.43
1:I:100(F):VAL:HA	3:A:94:ASN:HD22	1.83	0.43
3:A:84:ARG:HB3	3:A:103:GLN:HE22	1.83	0.43
4:D:715:ILE:O	4:D:942:GLU:HA	2.18	0.43
3:G:84:ARG:HB3	3:G:103:GLN:HE22	1.84	0.43
2:P:90:GLN:O	2:P:95:PHE:HA	2.19	0.43
4:D:691:ARG:NH1	4:D:1008:SER:H	2.17	0.43
3:E:84:ARG:HB3	3:E:103:GLN:HE22	1.83	0.43
3:E:138:ASN:HB3	3:E:323:PRO:HG3	2.01	0.43
2:N:32:VAL:HG12	2:N:91:ALA:H	1.84	0.42
3:A:185:ILE:HD13	3:A:208:VAL:HG11	2.01	0.42
4:H:976:LEU:HD11	4:H:1049:HIS:HB3	2.00	0.42
1:O:83:ARG:HB3	1:O:85:GLU:OE1	2.19	0.42
3:A:285:HIS:HB3	4:B:733:LYS:HZ1	1.83	0.42
4:B:976:LEU:HD11	4:B:1049:HIS:HB3	2.01	0.42
3:A:60:LEU:HD11	3:A:133:TYR:HD1	1.84	0.42
3:A:84:ARG:HD2	3:A:85:LYS:O	2.19	0.42
3:C:60:LEU:HD11	3:C:133:TYR:HD1	1.83	0.42
3:G:60:LEU:HD11	3:G:133:TYR:HD1	1.83	0.42
1:M:83:ARG:HB3	1:M:85:GLU:OE1	2.20	0.42
4:D:976:LEU:HD11	4:D:1049:HIS:HB3	2.00	0.42
3:C:84:ARG:HD2	3:C:85:LYS:O	2.19	0.42
3:E:185:ILE:HD13	3:E:208:VAL:HG11	2.02	0.42
4:F:710:MET:HE1	4:F:954:VAL:HG11	2.01	0.42
4:H:691:ARG:NH1	4:H:1008:SER:H	2.17	0.42
1:K:83:ARG:HB3	1:K:85:GLU:OE1	2.20	0.42
4:H:710:MET:HE1	4:H:954:VAL:HG11	2.01	0.42
3:A:234:LEU:HD23	3:A:234:LEU:HA	1.90	0.42
3:C:185:ILE:HD13	3:C:208:VAL:HG11	2.02	0.42
3:A:28:MET:HE3	3:A:28:MET:HB3	1.99	0.42
3:C:84:ARG:HB3	3:C:103:GLN:HE22	1.84	0.42
3:C:138:ASN:HB3	3:C:323:PRO:HG3	2.02	0.42
3:G:38:GLN:HB2	3:G:257:GLU:OE2	2.20	0.42
3:G:84:ARG:HD2	3:G:85:LYS:O	2.19	0.42
3:G:138:ASN:HB3	3:G:323:PRO:HG3	2.01	0.42
3:G:185:ILE:HD13	3:G:208:VAL:HG11	2.02	0.42
1:I:24:ALA:HB3	1:I:29:PHE:CE1	2.55	0.41
3:A:38:GLN:HB2	3:A:257:GLU:OE2	2.20	0.41
1:O:24:ALA:HB3	1:O:29:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:84:ARG:HD2	3:E:85:LYS:O	2.19	0.41
4:H:1026:ALA:N	4:H:1030:ASN:HD21	2.18	0.41
1:M:24:ALA:HB3	1:M:29:PHE:CE1	2.55	0.41
2:P:61:ARG:HG3	2:P:75:ILE:HG13	2.02	0.41
3:E:38:GLN:HB2	3:E:257:GLU:OE2	2.20	0.41
2:N:90:GLN:O	2:N:95:PHE:HA	2.20	0.41
3:A:287:ALA:HA	3:A:324:MET:HG2	2.03	0.41
3:A:116:ALA:HB3	3:A:119:LEU:HG	2.02	0.41
4:B:1026:ALA:N	4:B:1030:ASN:HD21	2.18	0.41
4:D:710:MET:HE1	4:D:954:VAL:HG11	2.03	0.41
3:A:69:HIS:CE1	3:A:119:LEU:HD21	2.56	0.41
3:C:116:ALA:HB3	3:C:119:LEU:HG	2.02	0.41
3:G:116:ALA:HB3	3:G:119:LEU:HG	2.02	0.41
3:G:287:ALA:HA	3:G:324:MET:HG2	2.03	0.41
4:B:710:MET:HE1	4:B:954:VAL:HG11	2.02	0.41
4:D:1026:ALA:N	4:D:1030:ASN:HD21	2.17	0.41
2:J:61:ARG:HG3	2:J:75:ILE:HG13	2.02	0.41
3:A:305:VAL:HG11	3:A:340:VAL:HG22	2.02	0.41
3:C:69:HIS:CE1	3:C:119:LEU:HD21	2.56	0.41
3:E:69:HIS:CE1	3:E:119:LEU:HD21	2.56	0.41
1:K:24:ALA:HB3	1:K:29:PHE:CE1	2.55	0.40
3:A:138:ASN:HB3	3:A:323:PRO:HG3	2.02	0.40
4:F:691:ARG:NH1	4:F:1008:SER:H	2.19	0.40
3:A:60:LEU:HD23	3:A:165:VAL:HG22	2.03	0.40
4:F:929:PHE:HE2	4:F:931:LEU:HD21	1.86	0.40
3:G:305:VAL:HG11	3:G:340:VAL:HG22	2.03	0.40
2:L:61:ARG:HG3	2:L:75:ILE:HG13	2.02	0.40
3:C:393:GLU:OE1	3:C:422:LYS:HG3	2.21	0.40
3:E:305:VAL:HG11	3:E:340:VAL:HG22	2.03	0.40
4:F:1026:ALA:N	4:F:1030:ASN:HD21	2.18	0.40
4:H:691:ARG:HH12	4:H:1008:SER:H	1.69	0.40
3:E:116:ALA:HB3	3:E:119:LEU:HG	2.02	0.40
3:G:69:HIS:CE1	3:G:119:LEU:HD21	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	113/126 (90%)	107 (95%)	6 (5%)	0	100	100
1	K	113/126 (90%)	107 (95%)	6 (5%)	0	100	100
1	M	113/126 (90%)	107 (95%)	6 (5%)	0	100	100
1	O	113/126 (90%)	107 (95%)	6 (5%)	0	100	100
2	J	106/111 (96%)	104 (98%)	2 (2%)	0	100	100
2	L	106/111 (96%)	104 (98%)	2 (2%)	0	100	100
2	N	106/111 (96%)	104 (98%)	2 (2%)	0	100	100
2	P	106/111 (96%)	104 (98%)	2 (2%)	0	100	100
3	A	458/651 (70%)	445 (97%)	13 (3%)	0	100	100
3	C	458/651 (70%)	444 (97%)	14 (3%)	0	100	100
3	E	458/651 (70%)	445 (97%)	13 (3%)	0	100	100
3	G	458/651 (70%)	445 (97%)	13 (3%)	0	100	100
4	B	429/609 (70%)	416 (97%)	13 (3%)	0	100	100
4	D	429/609 (70%)	416 (97%)	13 (3%)	0	100	100
4	F	429/609 (70%)	416 (97%)	13 (3%)	0	100	100
4	H	429/609 (70%)	416 (97%)	13 (3%)	0	100	100
All	All	4424/5988 (74%)	4287 (97%)	137 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	97/106 (92%)	97 (100%)	0	100	100
1	K	97/106 (92%)	97 (100%)	0	100	100
1	M	97/106 (92%)	97 (100%)	0	100	100
1	O	97/106 (92%)	97 (100%)	0	100	100
2	J	92/95 (97%)	92 (100%)	0	100	100
2	L	92/95 (97%)	92 (100%)	0	100	100
2	N	92/95 (97%)	92 (100%)	0	100	100
2	P	92/95 (97%)	92 (100%)	0	100	100
3	A	411/580 (71%)	411 (100%)	0	100	100
3	C	411/580 (71%)	411 (100%)	0	100	100
3	E	411/580 (71%)	411 (100%)	0	100	100
3	G	411/580 (71%)	411 (100%)	0	100	100
4	B	372/524 (71%)	372 (100%)	0	100	100
4	D	372/524 (71%)	372 (100%)	0	100	100
4	F	372/524 (71%)	372 (100%)	0	100	100
4	H	372/524 (71%)	372 (100%)	0	100	100
All	All	3888/5220 (74%)	3888 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	39	GLN
1	I	81	GLN
2	J	38	GLN
2	J	42	GLN
1	K	39	GLN
1	K	81	GLN
2	L	38	GLN
2	L	42	GLN
1	M	39	GLN
1	M	81	GLN
2	N	38	GLN
2	N	42	GLN
1	O	39	GLN
1	O	81	GLN

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Mol	Chain	Res	Type
2	P	38	GLN
2	P	42	GLN
3	A	65	ASN
3	A	94	ASN
3	A	255	HIS
3	A	454	GLN
4	B	955	ASN
4	B	1030	ASN
3	C	38	GLN
3	C	65	ASN
3	C	94	ASN
3	C	255	HIS
3	C	428	GLN
3	C	454	GLN
4	D	811	GLN
4	D	1030	ASN
3	E	65	ASN
3	E	255	HIS
3	E	454	GLN
4	F	955	ASN
4	F	1030	ASN
3	G	38	GLN
3	G	65	ASN
3	G	94	ASN
3	G	255	HIS
3	G	351	HIS
3	G	411	ASN
3	G	428	GLN
3	G	454	GLN
4	H	816	GLN
4	H	955	ASN
4	H	1024	ASN
4	H	1030	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

28 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	Q	1	3,5	14,14,15	0.78	0	17,19,21	1.21	2 (11%)
5	NAG	Q	2	5	14,14,15	0.71	0	17,19,21	0.87	1 (5%)
5	BMA	Q	3	5	11,11,12	0.80	0	15,15,17	2.50	4 (26%)
5	MAN	Q	4	5	11,11,12	0.71	0	15,15,17	1.07	1 (6%)
5	MAN	Q	5	5	11,11,12	0.77	0	15,15,17	0.95	1 (6%)
6	NAG	R	1	6,3	14,14,15	0.74	0	17,19,21	0.94	1 (5%)
6	NAG	R	2	6	14,14,15	0.73	0	17,19,21	0.97	0
5	NAG	S	1	3,5	14,14,15	0.75	0	17,19,21	1.22	2 (11%)
5	NAG	S	2	5	14,14,15	0.70	0	17,19,21	0.86	1 (5%)
5	BMA	S	3	5	11,11,12	0.81	0	15,15,17	2.50	4 (26%)
5	MAN	S	4	5	11,11,12	0.69	0	15,15,17	1.08	1 (6%)
5	MAN	S	5	5	11,11,12	0.75	0	15,15,17	0.97	1 (6%)
6	NAG	T	1	6,3	14,14,15	0.72	0	17,19,21	0.94	1 (5%)
6	NAG	T	2	6	14,14,15	0.74	0	17,19,21	0.97	0
5	NAG	U	1	3,5	14,14,15	0.76	0	17,19,21	1.22	2 (11%)
5	NAG	U	2	5	14,14,15	0.71	0	17,19,21	0.86	1 (5%)
5	BMA	U	3	5	11,11,12	0.83	0	15,15,17	2.50	4 (26%)
5	MAN	U	4	5	11,11,12	0.71	0	15,15,17	1.09	1 (6%)
5	MAN	U	5	5	11,11,12	0.76	0	15,15,17	0.98	1 (6%)
6	NAG	V	1	6,3	14,14,15	0.75	0	17,19,21	0.94	1 (5%)
6	NAG	V	2	6	14,14,15	0.72	0	17,19,21	0.97	0
5	NAG	W	1	3,5	14,14,15	0.76	0	17,19,21	1.22	2 (11%)
5	NAG	W	2	5	14,14,15	0.71	0	17,19,21	0.86	1 (5%)
5	BMA	W	3	5	11,11,12	0.82	0	15,15,17	2.51	4 (26%)
5	MAN	W	4	5	11,11,12	0.69	0	15,15,17	1.08	1 (6%)
5	MAN	W	5	5	11,11,12	0.76	0	15,15,17	0.98	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	X	1	6,3	14,14,15	0.73	0	17,19,21	0.92	1 (5%)
6	NAG	X	2	6	14,14,15	0.74	0	17,19,21	0.96	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	Q	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	0/6/23/26	0/1/1/1
5	BMA	Q	3	5	-	1/2/19/22	0/1/1/1
5	MAN	Q	4	5	-	0/2/19/22	1/1/1/1
5	MAN	Q	5	5	-	2/2/19/22	0/1/1/1
6	NAG	R	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	R	2	6	-	0/6/23/26	0/1/1/1
5	NAG	S	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	S	2	5	-	0/6/23/26	0/1/1/1
5	BMA	S	3	5	-	1/2/19/22	0/1/1/1
5	MAN	S	4	5	-	0/2/19/22	1/1/1/1
5	MAN	S	5	5	-	2/2/19/22	0/1/1/1
6	NAG	T	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	T	2	6	-	0/6/23/26	0/1/1/1
5	NAG	U	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	U	2	5	-	0/6/23/26	0/1/1/1
5	BMA	U	3	5	-	1/2/19/22	0/1/1/1
5	MAN	U	4	5	-	0/2/19/22	1/1/1/1
5	MAN	U	5	5	-	2/2/19/22	0/1/1/1
6	NAG	V	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	V	2	6	-	0/6/23/26	0/1/1/1
5	NAG	W	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	W	2	5	-	0/6/23/26	0/1/1/1
5	BMA	W	3	5	-	1/2/19/22	0/1/1/1
5	MAN	W	4	5	-	0/2/19/22	1/1/1/1
5	MAN	W	5	5	-	2/2/19/22	0/1/1/1
6	NAG	X	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	X	2	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	W	3	BMA	C1-O5-C5	7.83	122.68	112.19
5	S	3	BMA	C1-O5-C5	7.82	122.67	112.19
5	U	3	BMA	C1-O5-C5	7.80	122.64	112.19
5	Q	3	BMA	C1-O5-C5	7.79	122.63	112.19
5	S	4	MAN	C1-O5-C5	3.01	116.22	112.19
5	W	3	BMA	C3-C4-C5	3.01	115.68	110.23
5	Q	4	MAN	C1-O5-C5	2.99	116.19	112.19
5	U	4	MAN	C1-O5-C5	2.99	116.19	112.19
5	W	4	MAN	C1-O5-C5	2.99	116.19	112.19
5	U	3	BMA	C3-C4-C5	2.98	115.64	110.23
5	Q	3	BMA	C3-C4-C5	2.96	115.60	110.23
5	S	3	BMA	C3-C4-C5	2.96	115.59	110.23
5	Q	3	BMA	C2-C3-C4	2.49	115.25	110.86
5	W	3	BMA	C2-C3-C4	2.49	115.24	110.86
5	S	3	BMA	C2-C3-C4	2.48	115.23	110.86
5	U	3	BMA	C2-C3-C4	2.46	115.19	110.86
5	U	5	MAN	C1-O5-C5	2.40	115.40	112.19
5	W	5	MAN	C1-O5-C5	2.37	115.36	112.19
6	V	1	NAG	C2-N2-C7	2.31	126.00	122.90
6	T	1	NAG	C2-N2-C7	2.29	125.97	122.90
5	S	1	NAG	C1-O5-C5	2.29	115.25	112.19
5	W	1	NAG	C1-O5-C5	2.28	115.24	112.19
5	S	5	MAN	C1-O5-C5	2.28	115.24	112.19
6	R	1	NAG	C2-N2-C7	2.27	125.94	122.90
5	U	1	NAG	C1-O5-C5	2.27	115.22	112.19
6	X	1	NAG	C2-N2-C7	2.25	125.92	122.90
5	Q	1	NAG	C1-O5-C5	2.22	115.16	112.19
5	Q	5	MAN	C1-O5-C5	2.20	115.14	112.19
5	U	3	BMA	O4-C4-C3	-2.18	105.25	110.38
5	W	3	BMA	O4-C4-C3	-2.17	105.27	110.38
5	S	3	BMA	O4-C4-C3	-2.16	105.28	110.38
5	Q	3	BMA	O4-C4-C3	-2.14	105.32	110.38
5	Q	2	NAG	O5-C1-C2	-2.08	108.07	111.29
5	U	2	NAG	O5-C1-C2	-2.07	108.10	111.29
5	U	1	NAG	C2-N2-C7	2.06	125.67	122.90
5	W	2	NAG	O5-C1-C2	-2.05	108.12	111.29
5	S	2	NAG	O5-C1-C2	-2.05	108.13	111.29
5	Q	1	NAG	C2-N2-C7	2.02	125.60	122.90
5	S	1	NAG	C2-N2-C7	2.02	125.60	122.90
5	W	1	NAG	C2-N2-C7	2.01	125.60	122.90

There are no chirality outliers.

All (20) torsion outliers are listed below:

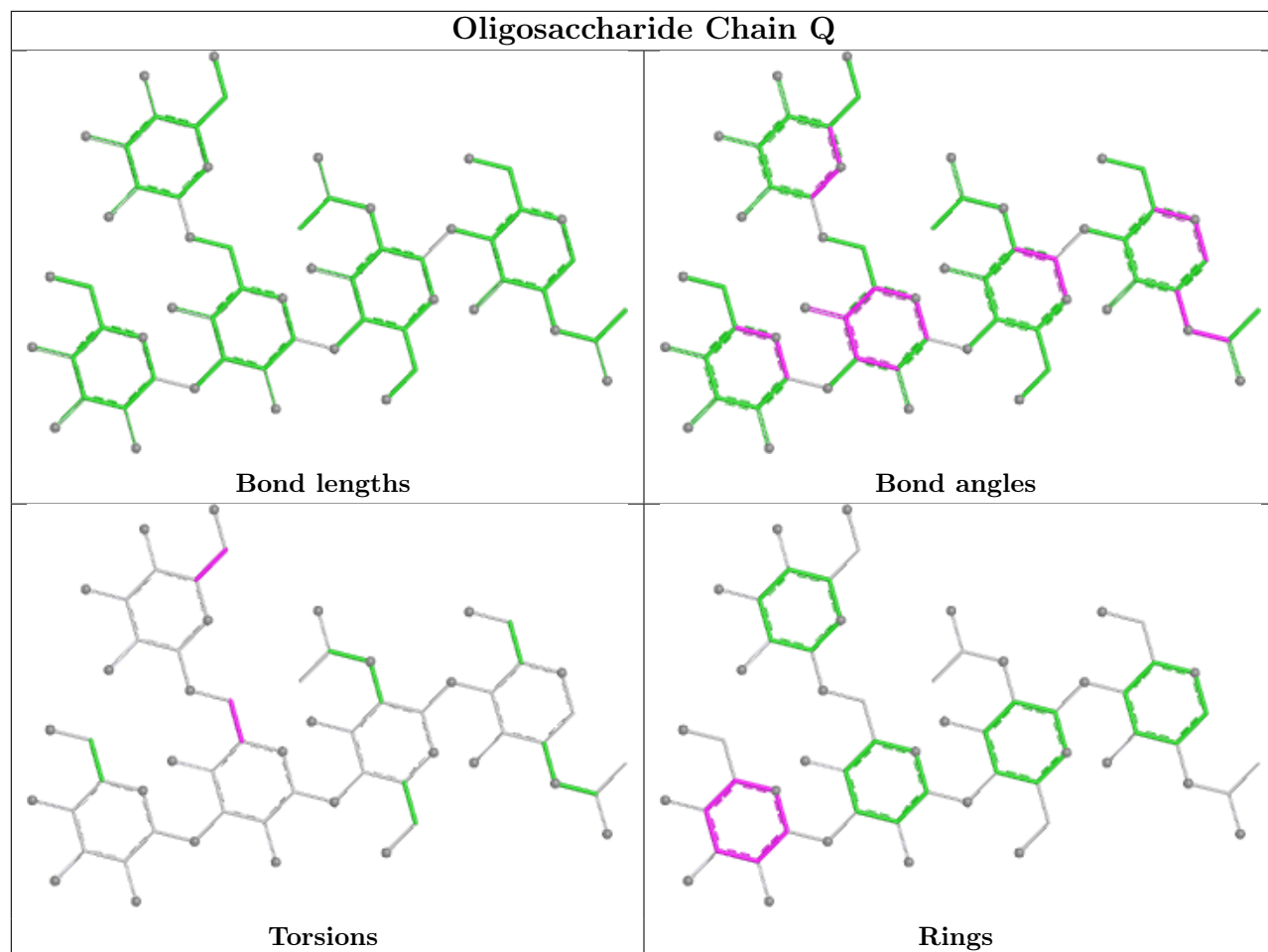
Mol	Chain	Res	Type	Atoms
5	Q	5	MAN	O5-C5-C6-O6
5	S	5	MAN	O5-C5-C6-O6
5	U	5	MAN	O5-C5-C6-O6
5	W	5	MAN	O5-C5-C6-O6
5	Q	5	MAN	C4-C5-C6-O6
5	S	5	MAN	C4-C5-C6-O6
5	U	5	MAN	C4-C5-C6-O6
5	W	5	MAN	C4-C5-C6-O6
6	R	1	NAG	C8-C7-N2-C2
6	R	1	NAG	O7-C7-N2-C2
6	T	1	NAG	C8-C7-N2-C2
6	T	1	NAG	O7-C7-N2-C2
6	V	1	NAG	C8-C7-N2-C2
6	V	1	NAG	O7-C7-N2-C2
6	X	1	NAG	C8-C7-N2-C2
6	X	1	NAG	O7-C7-N2-C2
5	U	3	BMA	O5-C5-C6-O6
5	W	3	BMA	O5-C5-C6-O6
5	Q	3	BMA	O5-C5-C6-O6
5	S	3	BMA	O5-C5-C6-O6

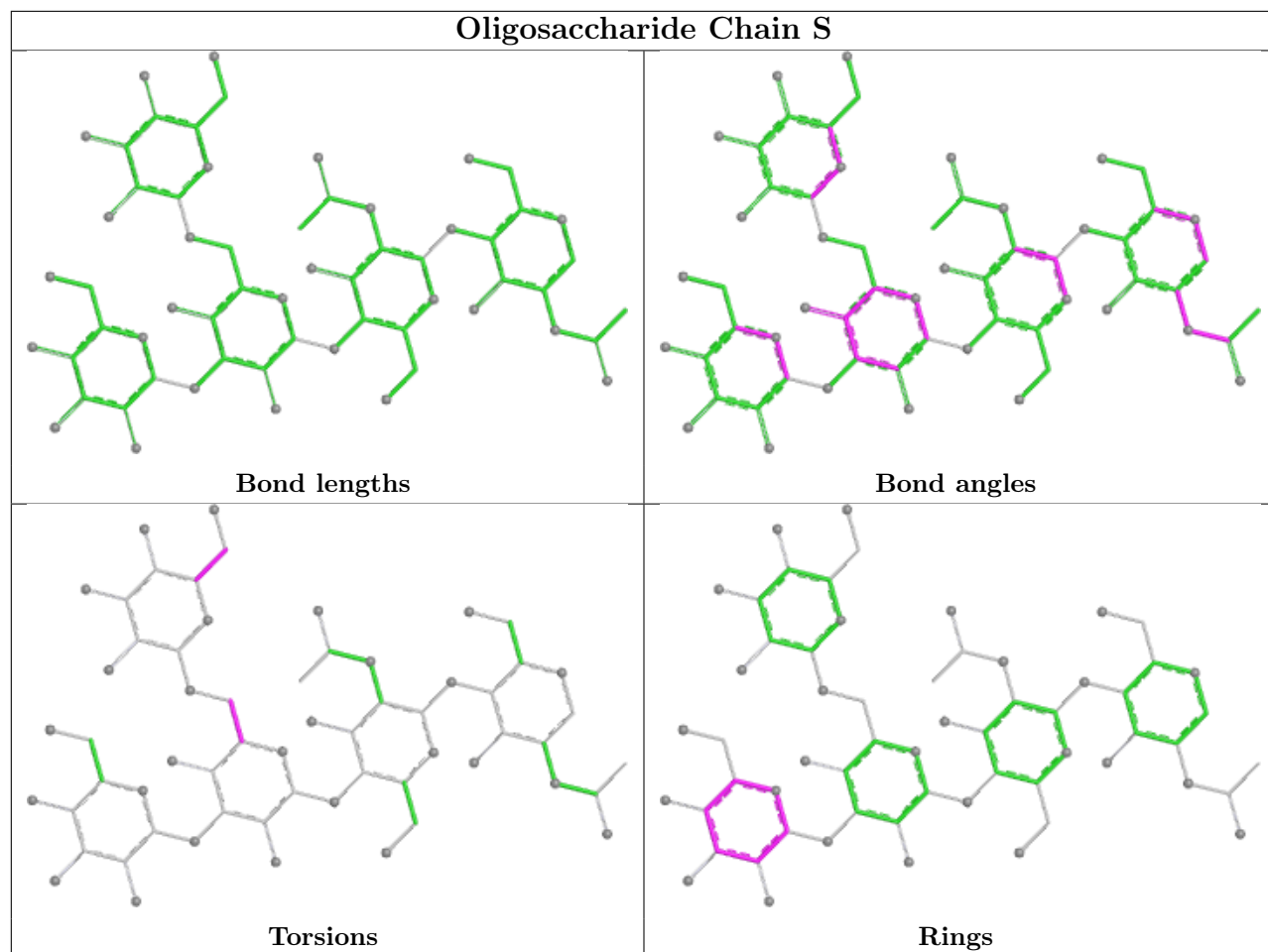
All (4) ring outliers are listed below:

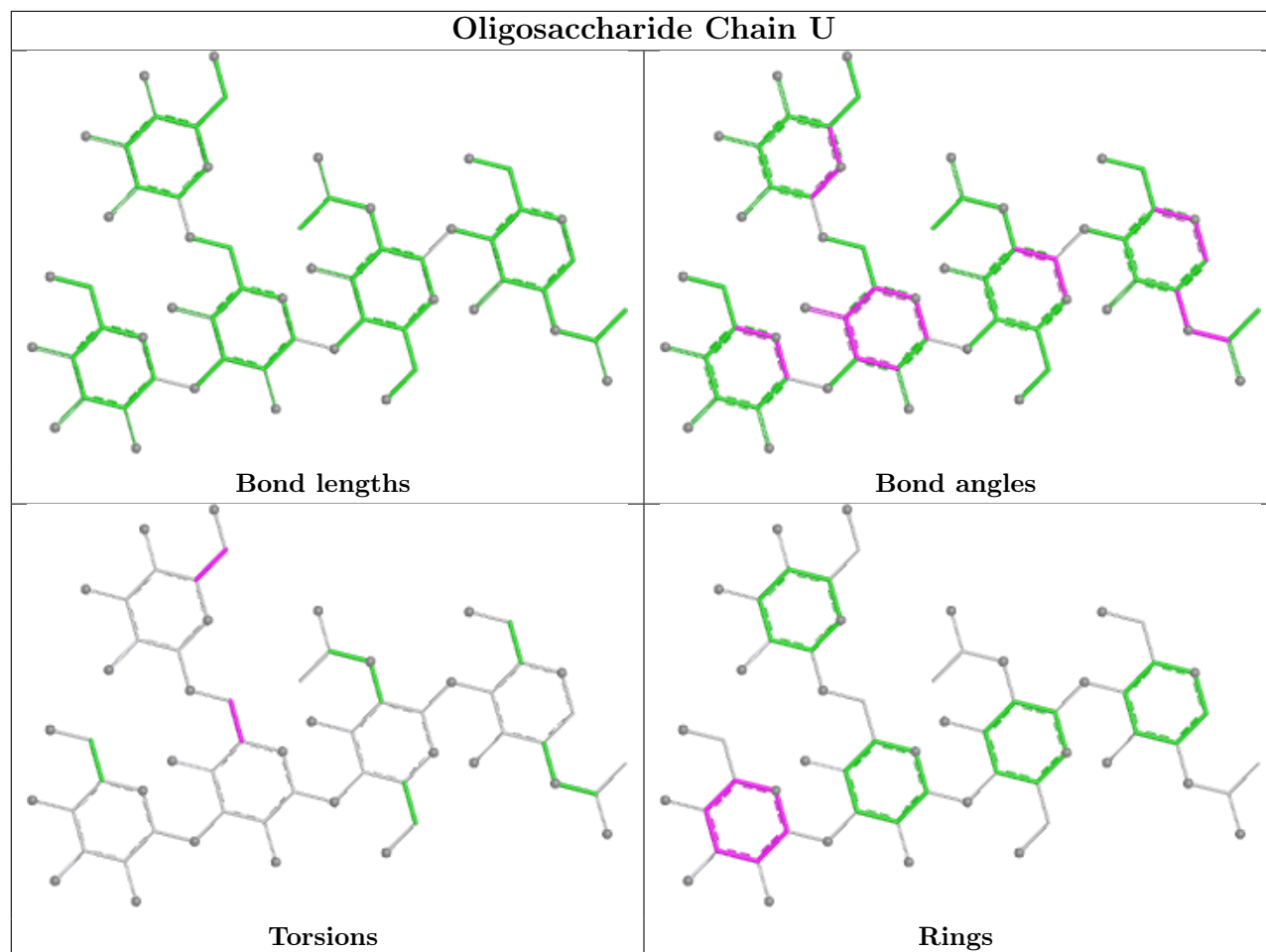
Mol	Chain	Res	Type	Atoms
5	Q	4	MAN	C1-C2-C3-C4-C5-O5
5	W	4	MAN	C1-C2-C3-C4-C5-O5
5	U	4	MAN	C1-C2-C3-C4-C5-O5
5	S	4	MAN	C1-C2-C3-C4-C5-O5

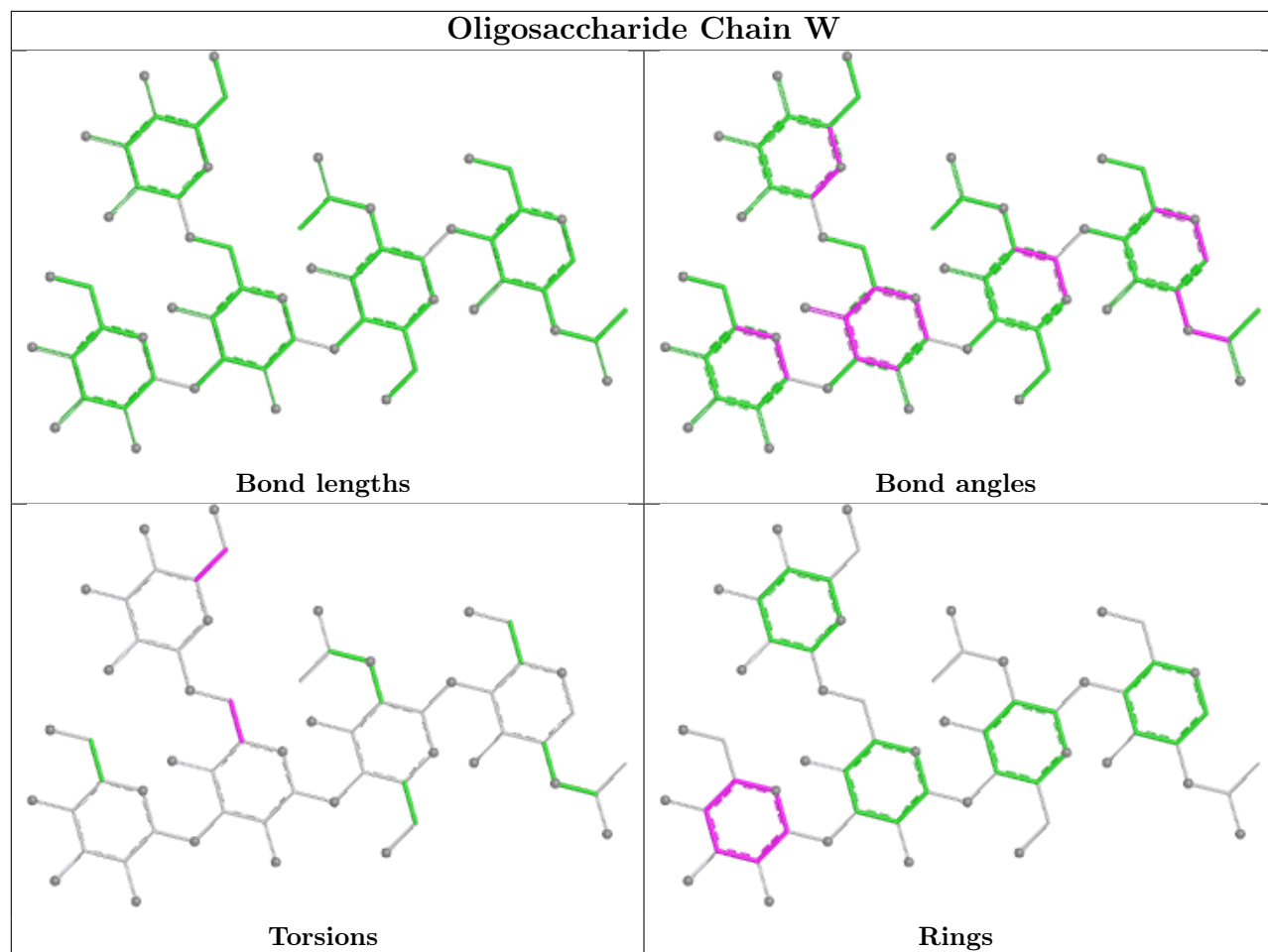
No monomer is involved in short contacts.

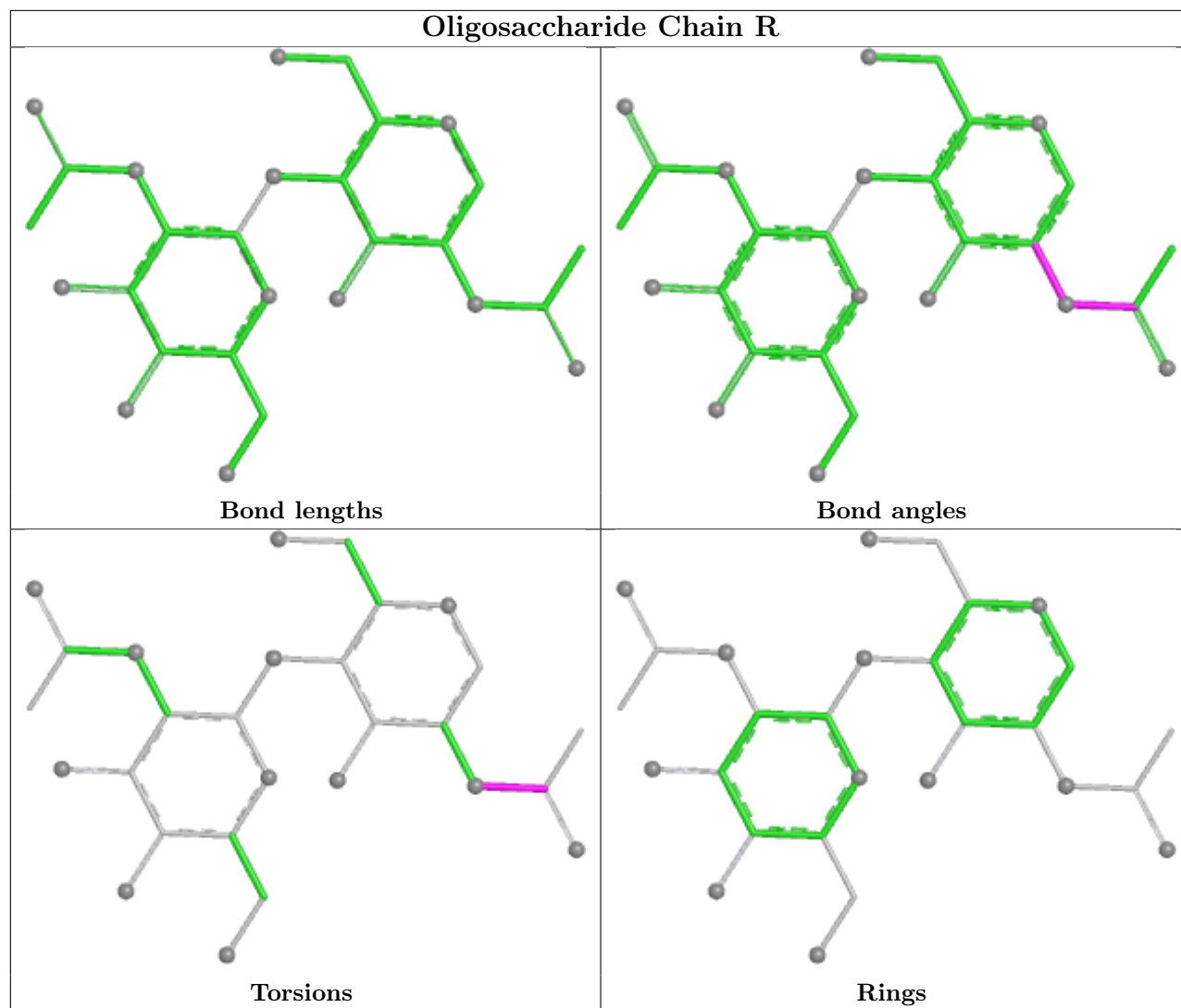
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

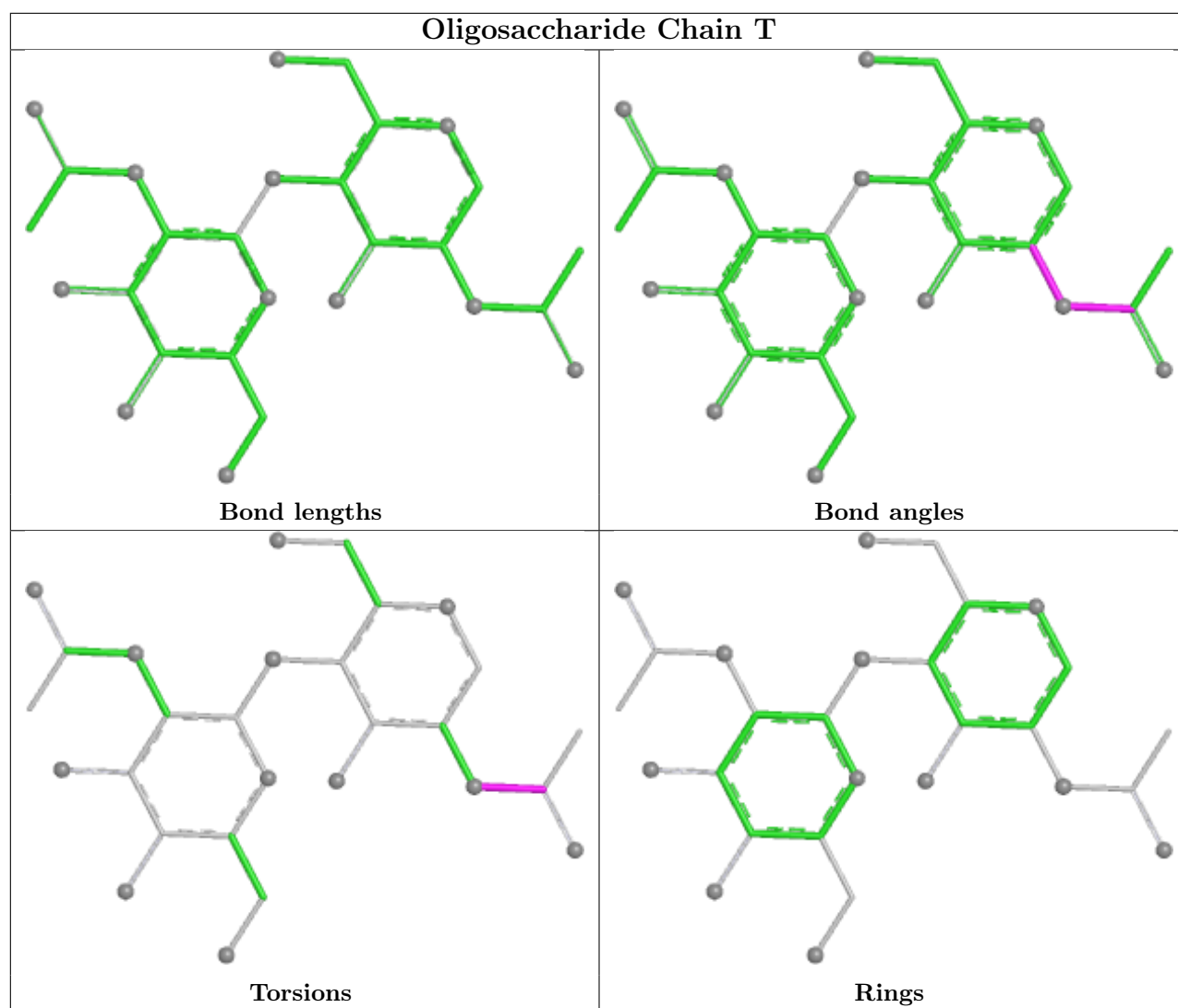


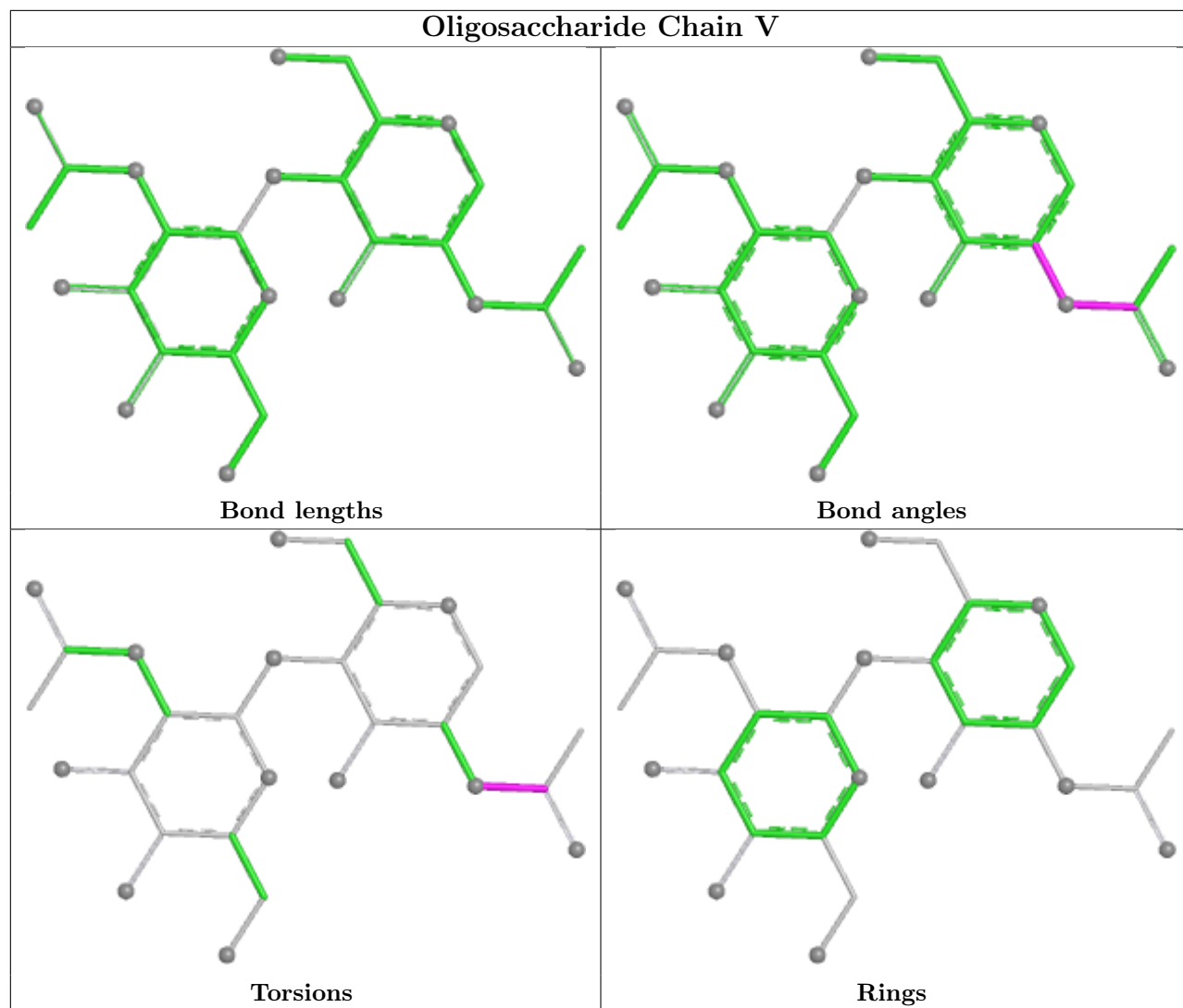


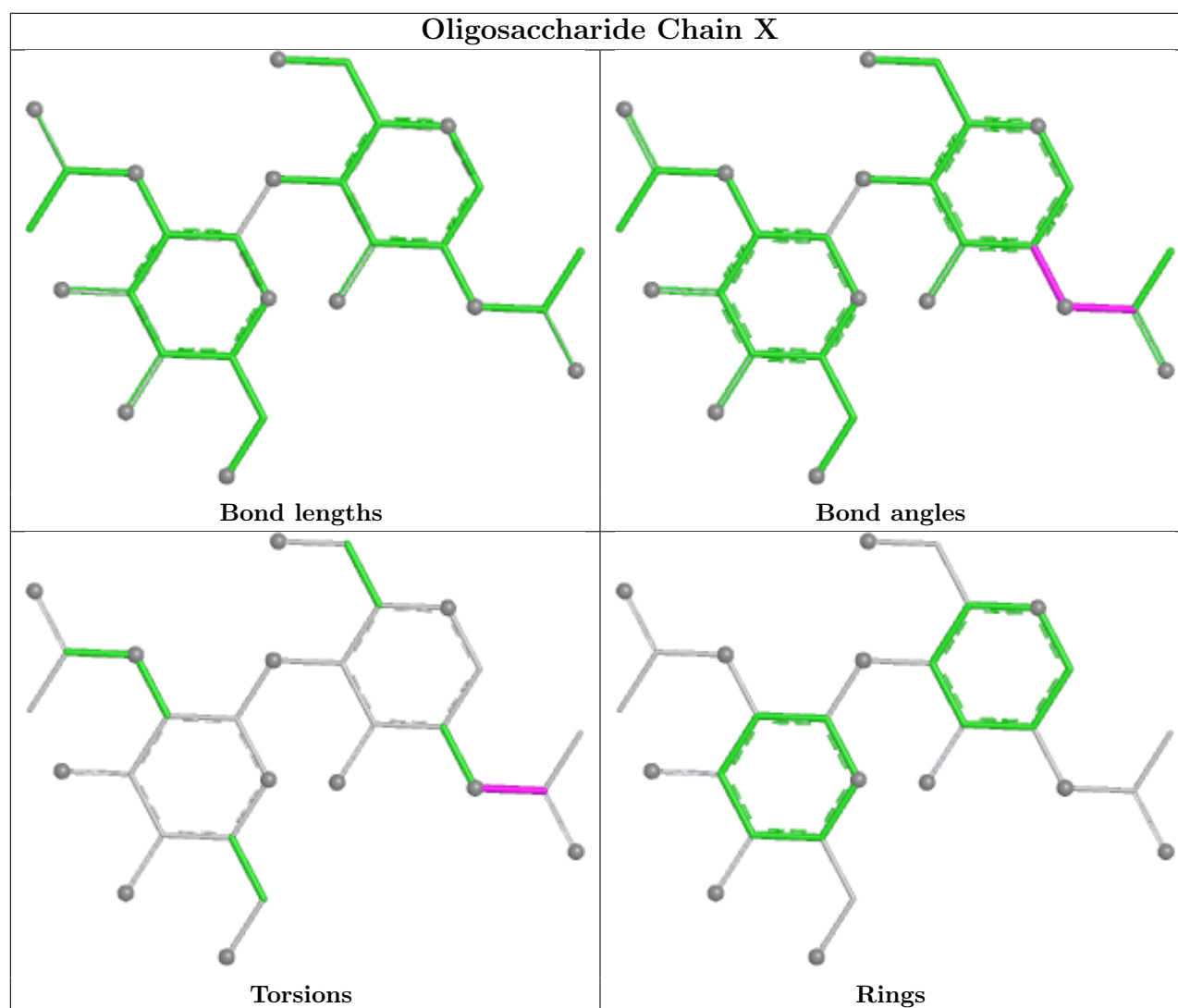












5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	G	701	3	14,14,15	0.76	0	17,19,21	1.35	1 (5%)
7	NAG	A	701	3	14,14,15	0.77	0	17,19,21	1.35	1 (5%)
7	NAG	E	701	3	14,14,15	0.77	0	17,19,21	1.35	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	C	701	3	14,14,15	0.76	0	17,19,21	1.36	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	G	701	3	-	2/6/23/26	0/1/1/1
7	NAG	A	701	3	-	2/6/23/26	0/1/1/1
7	NAG	E	701	3	-	2/6/23/26	0/1/1/1
7	NAG	C	701	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	701	NAG	C2-N2-C7	3.84	128.04	122.90
7	G	701	NAG	C2-N2-C7	3.81	128.01	122.90
7	E	701	NAG	C2-N2-C7	3.81	128.00	122.90
7	A	701	NAG	C2-N2-C7	3.80	127.99	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	701	NAG	C8-C7-N2-C2
7	A	701	NAG	O7-C7-N2-C2
7	C	701	NAG	C8-C7-N2-C2
7	C	701	NAG	O7-C7-N2-C2
7	E	701	NAG	C8-C7-N2-C2
7	E	701	NAG	O7-C7-N2-C2
7	G	701	NAG	C8-C7-N2-C2
7	G	701	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

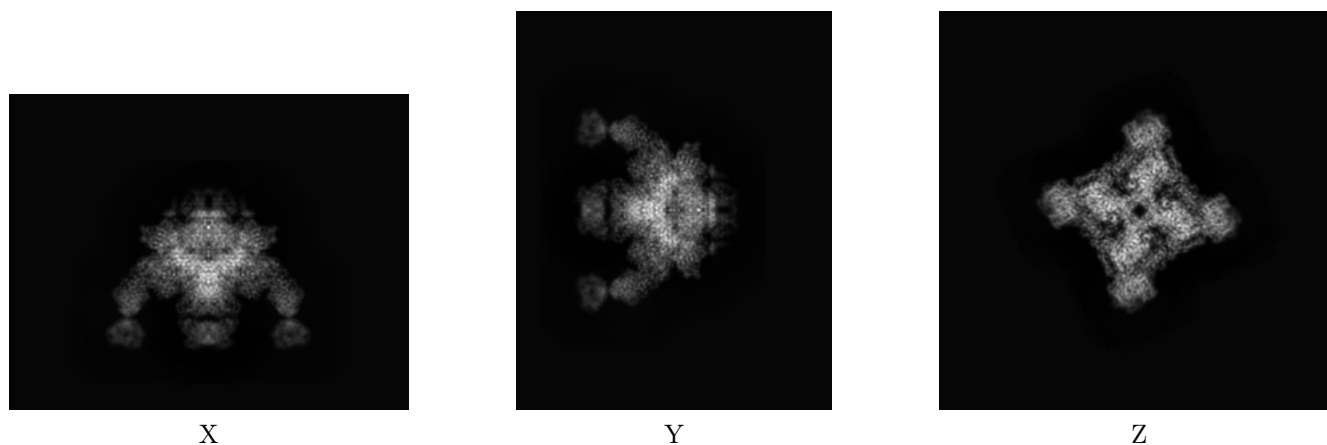
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71259. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

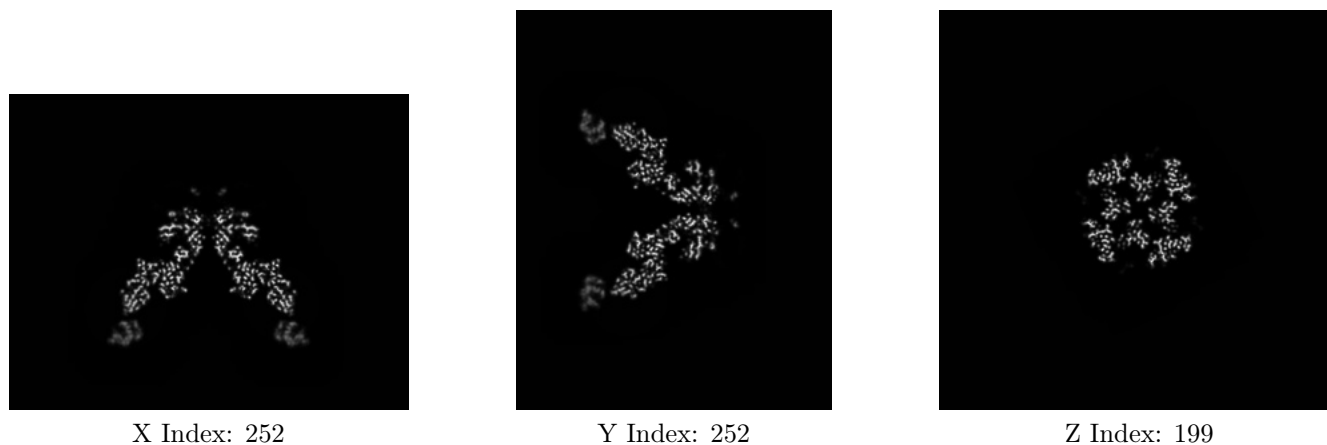
6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

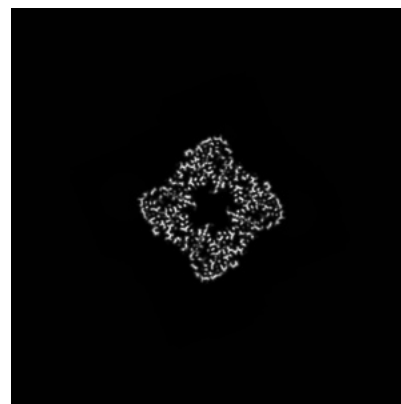
6.3.1 Primary map



X Index: 258



Y Index: 245

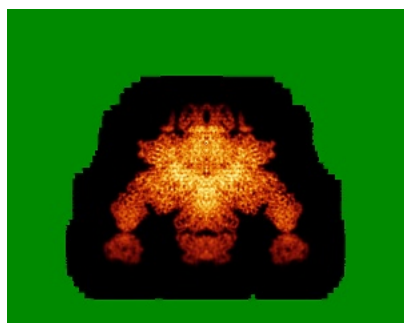


Z Index: 183

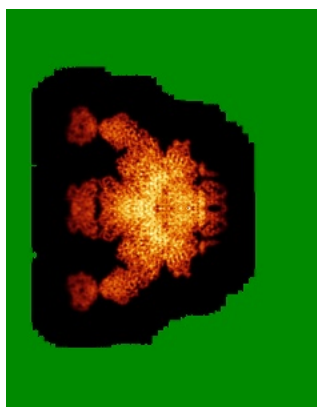
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

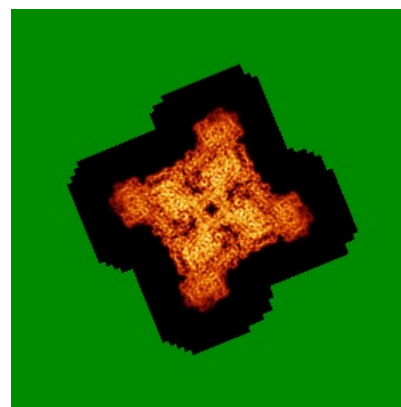
6.4.1 Primary map



X



Y

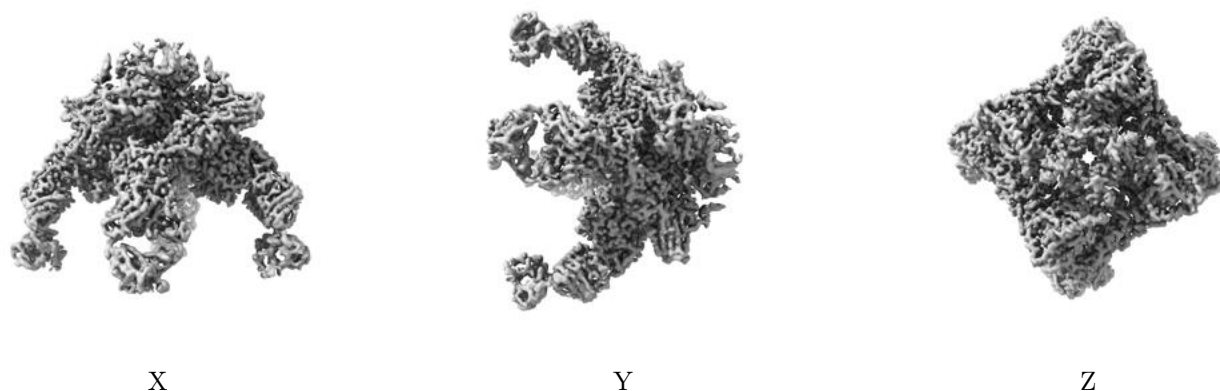


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

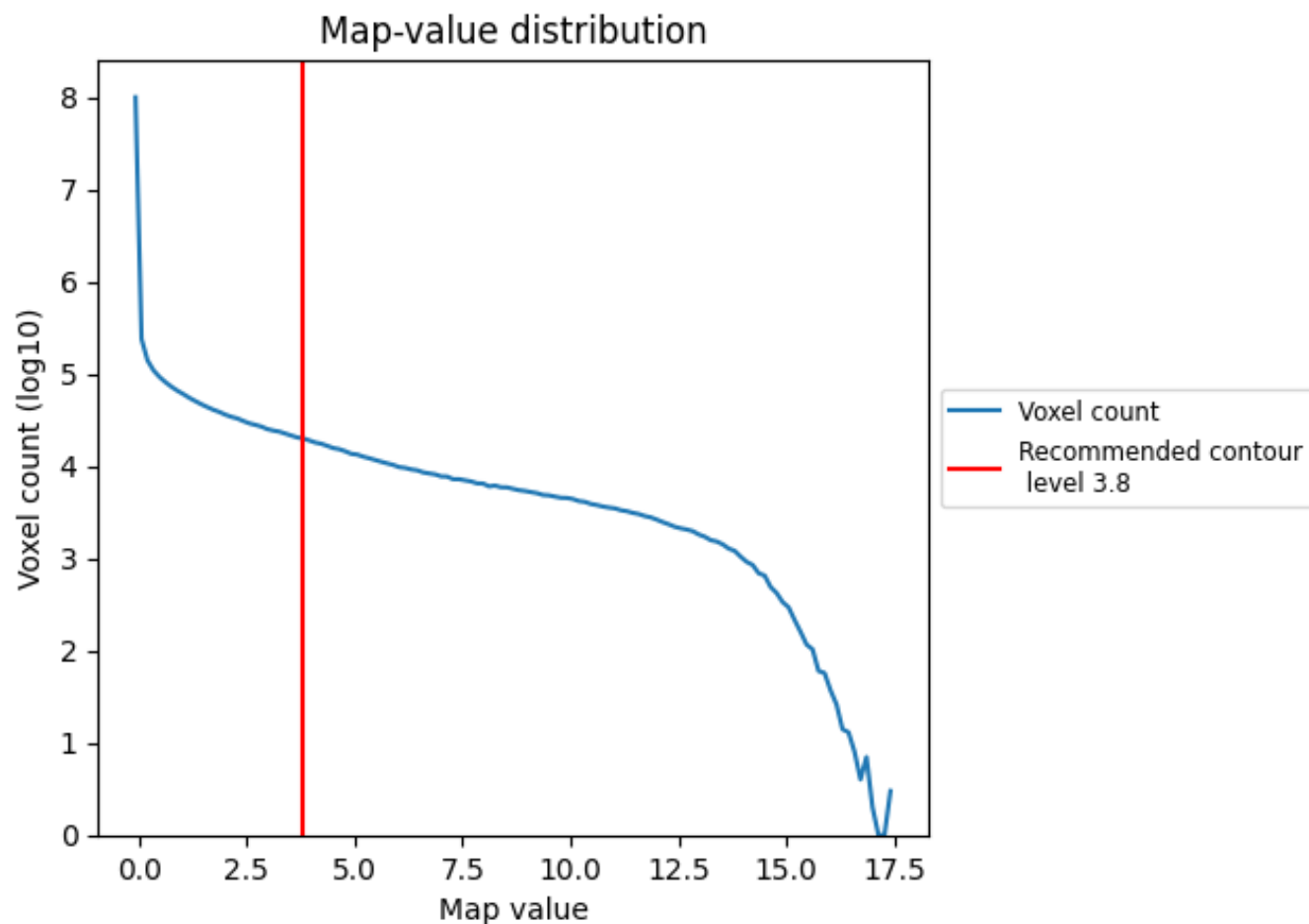
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

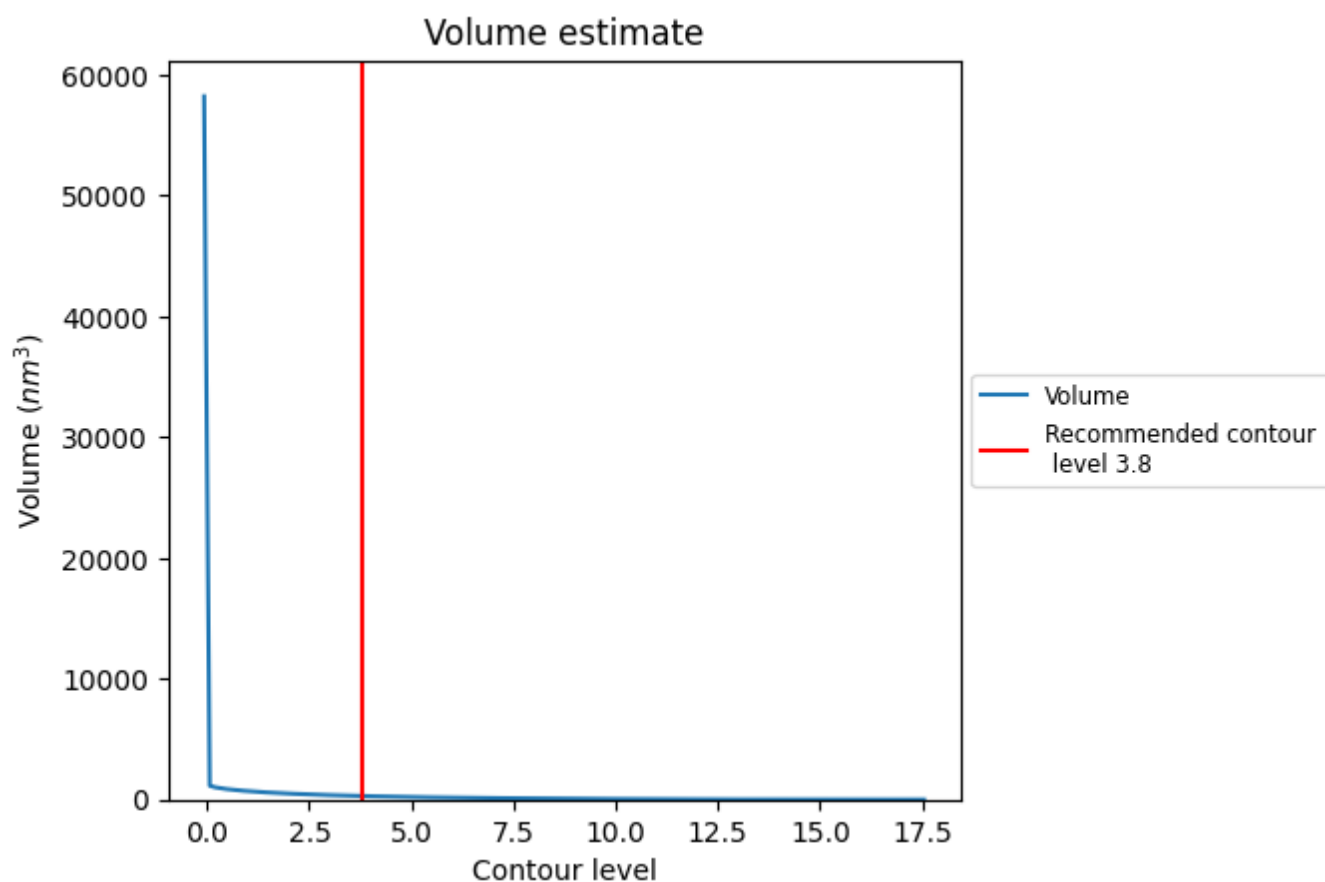
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 292 nm³; this corresponds to an approximate mass of 264 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

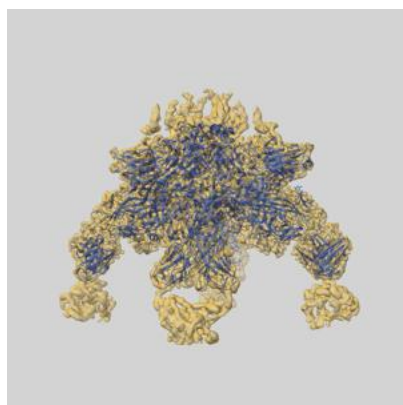
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

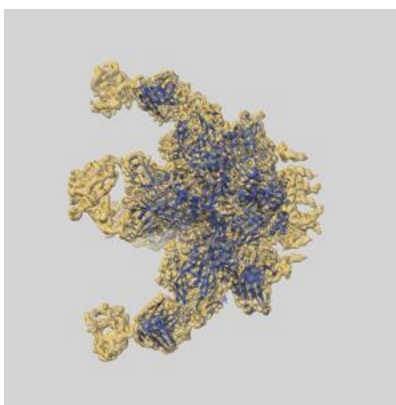
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71259 and PDB model 9P3Y. Per-residue inclusion information can be found in section [3](#) on page [19](#).

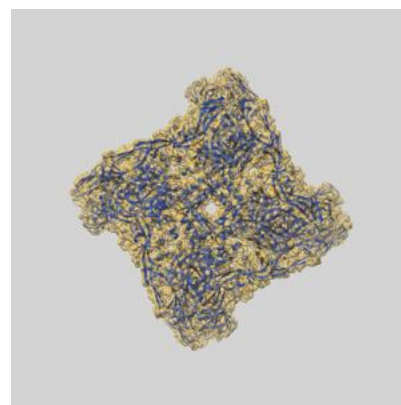
9.1 Map-model overlay [i](#)



X



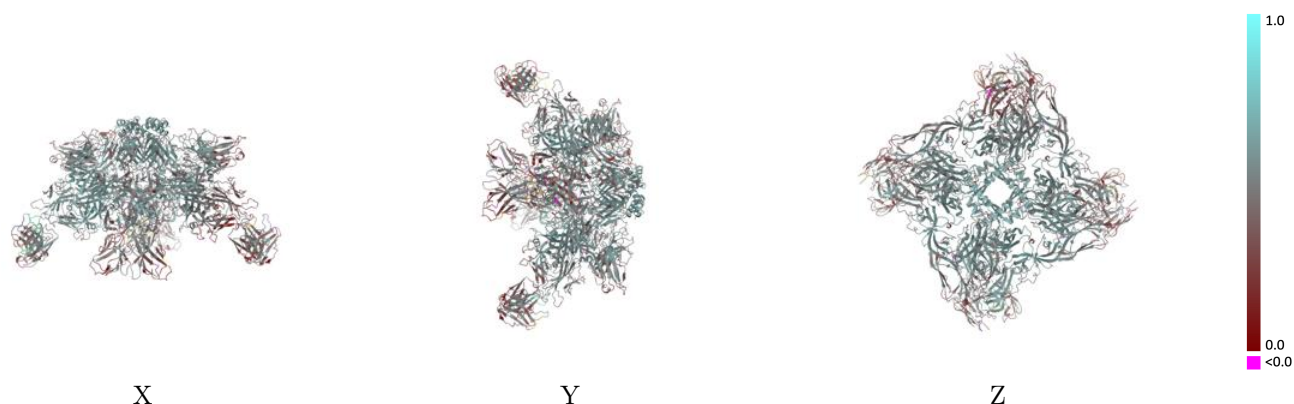
Y



Z

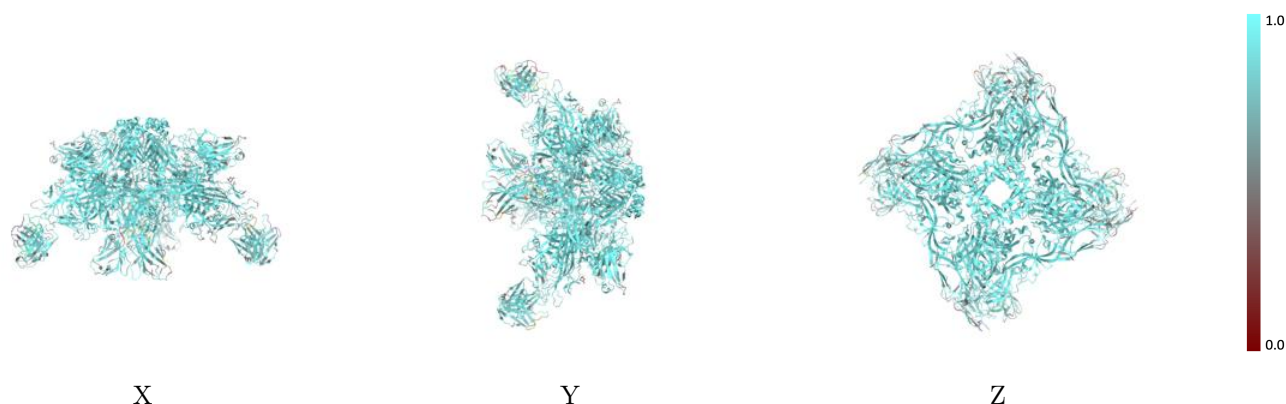
The images above show the 3D surface view of the map at the recommended contour level 3.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



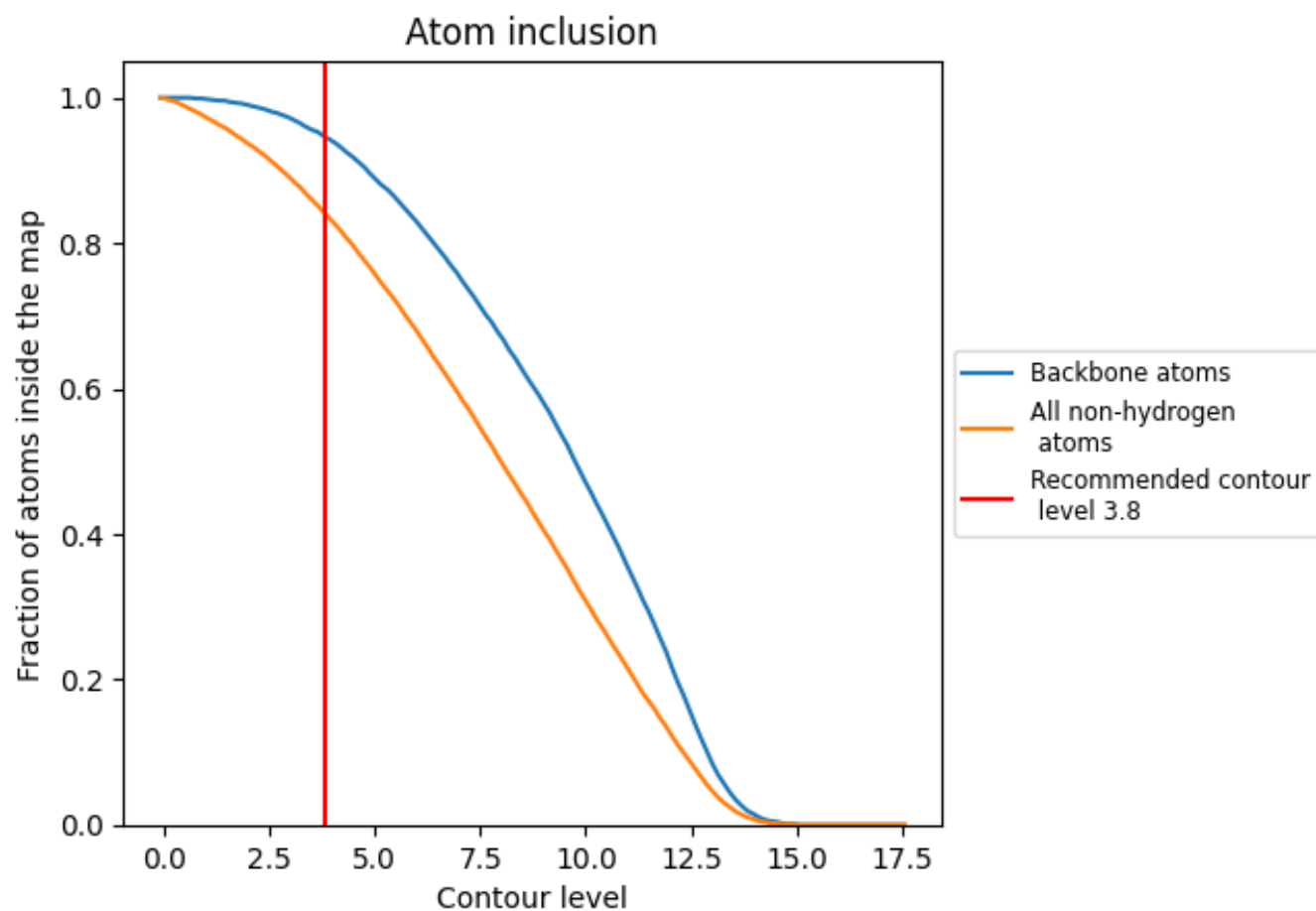
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8420	 0.4780
A	 0.9040	 0.5520
B	 0.8750	 0.5170
C	 0.8840	 0.5170
D	 0.8410	 0.4700
E	 0.8560	 0.4710
F	 0.8260	 0.4480
G	 0.8880	 0.5240
H	 0.8590	 0.4920
I	 0.7820	 0.4440
J	 0.7530	 0.4100
K	 0.7440	 0.3880
L	 0.7410	 0.3890
M	 0.7420	 0.3710
N	 0.7410	 0.3970
O	 0.7330	 0.3710
P	 0.7440	 0.3930
Q	 0.8360	 0.4720
R	 0.8570	 0.4430
S	 0.7380	 0.4510
T	 0.7500	 0.3180
U	 0.6720	 0.3830
V	 0.6070	 0.1850
W	 0.7210	 0.4260
X	 0.7500	 0.3660

